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FILE COVERS 1907 - 28 Oct 2005 VOL 143 ISS 19 FILE LAST UPDATED: 27 Oct 2005 (20051027/ED)

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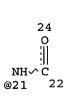
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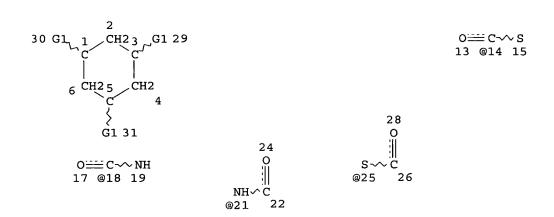
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STEREO ATTRIBUTES: NONE

56598 SEA FILE=REGISTRY SSS FUL L12 L14

L17 STR



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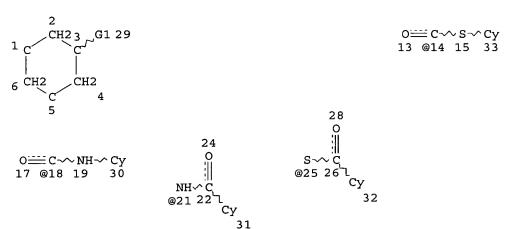
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STEREO ATTRIBUTES: NONE

L18 167 SEA FILE=REGISTRY SUB=L14 SSS FUL L17

L20 STR



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GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

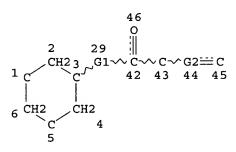
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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L22 STR



VAR G1=S/N REP G2=(0-20) C NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 12

101.00.10

STEREO ATTRIBUTES: NONE L23 145 SEA FILE=REGISTRY SUB=L18 SSS FUL L21 OR L22 OR L20

L24 60 SEA FILE=HCAPLUS ABB=ON PLU=ON L23

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L24 ANSWER 1 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:699419 HCAPLUS

DOCUMENT NUMBER: 143:311628

### Pryor 09 666463

TITLE: Two-stage enzyme mediated drug release from LMWG

hydrogels

AUTHOR(S): Van Bommel, Kjeld J. C.; Stuart, Marc C. A.; Feringa,

Ben L.; Van Esch, Jan

CORPORATE SOURCE: Biomade Technology Foundation, Nijenborgh, 4, 9747 AG,

Neth.

SOURCE: Organic & Biomolecular Chemistry (2005), 3(16),

2917-2920

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

AB An enzymically cleavable low mol. weight gelator-(model) drug conjugate system can be employed to effect a two-step enzyme mediated drug release, demonstrating the potential of LMWG systems for the development of drug

delivery devices.

IT 800373-95-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(two-stage enzyme mediated drug release from LMWG hydrogels)

RN 800373-95-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-

[(1S)-2-oxo-1-(phenylmethyl)-2-(6-quinolinylamino)ethyl]-,

 $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:503961 HCAPLUS

DOCUMENT NUMBER: 143:7602

TITLE: New polydentate chelating agents of the

3-hydroxy-4-pyridinone type, and their pharmaceutical

and environmental applications

INVENTOR(S): Seabra, Maria Amelia Loureiro dos Santos; Grazina,

Raquel Eliana Lourenco; Gano, Maria de Lurdes Barrela

Patricio; Gama, Ana Sofia Cavalheiro

PATENT ASSIGNEE(S): Instituto Superior Tecnico, Port.

SOURCE: Port. Pat. Appl., 48 pp.

CODEN: PTXXB9

DOCUMENT TYPE: Patent
LANGUAGE: Portuguese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

## Pryor 09 666463

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PT 102660	A	20030228	PT 2001-102660	20010821
PT 102660	В	20040227		
PRIORITY APPLN. INFO.:			PT 2001-102660	20010821
OTHER SOURCE(S):	MARPAT	143:7602		
GT				

#### \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The invention discloses new polydentate chelating agents which contain two or more bidentate 3-hydroxy-4-pyridinone (3,4-HP) units, and which are based on monomeric or polymeric frameworks. Specifically, compds. containing bidentate units I are claimed [wherein: n = 3-5; R1 = H or C1-6 aliphatic hydrocarbyl in which one H atom may be substituted with OH or alkoxy; R2 = H or C1-6 aliphatic hydrocarbyl; R3 = H, C1-6 aliphatic hydrocarbyl, or aryl]. The new chelating agents have potential pharmaceutical and environmental applications. The compds. offer a wide variety of mol. supports and substitutions on the chelating units, as well as the possibility of strategically chosen spacer groups between them. Because of their high affinity and specificity for a series of metal ions at neutral or acid pH, good lipo-hydrophilic balance, and the absence of toxicity (no data), the compds. offer promise in oral or injectable chelation therapy of metal intoxication, or as radiodiagnostic agents. Among the monomer-supported chelating agents, those with two or three 3,4-HP groups coupled via amide linkages to a cyclohexanetricarboxylic acid skeleton are notable, as are polymeric chelating agents using polymeric supports, e.g., Sepharose or agarose. These compds. have a high capacity for sequestration or removal of traces of heavy metals from aqueous or plasmatic media, e.g., in extracorporeal decontamination. For instance, cis,cis-1,3,5-tricarboxy-1,3,5-trimethylcyclohexane (Kemp's acid) was treated with oxalyl chloride and DMF catalyst to give 85% of the corresponding monoanhydride-mono-acid chloride. Double amidation of the latter with over 4-fold excess 1-(3-aminopropyl)-3-(benzyloxy)-2-methyl-4-pyridinone (48%) followed by hydrogenolysis of the benzyl groups (80%) gave ligand II. The similarly prepared ligand III was studied in its interaction with the trivalent hard metal ions Al3+, Fe3+, and Ga+, with obtained values at physiol. pH being: pAl = 17.2, pFe = 25.8, and pGa = 21.1. In a partitioning test (octanol vs. aqueous Tris buffer at pH 7.4), the hexadentate analog of II and ligand III had distribution coeffs. D = 0.04 and 0.03, resp. In vivo assays showed that administration of III strongly increased excretion of 67Ga from mice, with the 24-h excreted value from 1/2 h-delayed administration (92.4%) being almost as much as that from simultaneous administration (96.2%) or from pre-formed chelate (97.4%), vs. 67Ga citrate control (35.0%). Two polymer-based chelating agents were prepared, one using Sepharose 6B support and CNBr linker, and the other using Sepharose 4B support and epichlorohydrin linker, both with 1-(3-aminopropyl)-3-hydroxy-2-methyl-4-pyridinone as the ligand monomer. The polymer was stable to loss of ligand in water at physiol. pH over 24 h, and showed a ligand monomer d. of 366  $\mu$ mol/g. When used to complex Fe3+ at pH 3, the polymer had a capacity of 327  $\mu$ mol/g.

IT 852200-56-7P

RL: BSU (Biological study, unclassified); CPS (Chemical process); DGN (Diagnostic use); PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(chelating agent; preparation, metal-complexation, and biol. applications of polydentate 3-hydroxy-4-pyridinone derivative chelating agents)

RN 852200-56-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[3-(3-hydroxy-2-methyl-4-oxo1(4H)-pyridinyl)propyl]-1,3,5-trimethyl-, (1α,3α,5α)(9CI) (CA INDEX NAME)

Relative stereochemistry.

$$(CH_2)_3$$
 $(CH_2)_3$ 
 $(CH_2)_3$ 

## IT 852200-57-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation, metal-complexation, and biol. applications of polydentate 3-hydroxy-4-pyridinone derivative chelating agents)

RN 852200-57-8 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-tris[3-[2-methyl-4-oxo-3-(phenylmethoxy)-1(4H)-pyridinyl]propyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

\_\_ Ph

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L24 ANSWER 3 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
                                   2005:451342 HCAPLUS
ACCESSION NUMBER:
                                   143:8826
DOCUMENT NUMBER:
                                   Preparation of nonsymmetrical gelling agents useful
TITLE:
                                   for pharmaceuticals, cosmetics, chromatography
                                   materials, and catalytically active materials
                                   Van Bommel, Kjeld Jacobus Cornelis; Van Esch, Johannes
INVENTOR(S):
                                   Henricus
                                   Applied Nano Systems B. V., Neth.
PATENT ASSIGNEE(S):
SOURCE:
                                   PCT Int. Appl., 69 pp.
                                   CODEN: PIXXD2
DOCUMENT TYPE:
                                   Patent
LANGUAGE:
                                   English
FAMILY ACC. NUM. COUNT:
                                   1
PATENT INFORMATION:
       PATENT NO.
                                   KIND
                                             DATE
                                                              APPLICATION NO.
       _____
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                                                                                               _____
                                                            WO 2004-NL723
      WO 2005047231
                                    A1
                                             20050526
                                                                                               20041014

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

                 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
PRIORITY APPLN. INFO.:
                                                              EP 2003-78599
                                                                                           A 20031112
OTHER SOURCE(S):
                                   MARPAT 143:8826
       The present invention relates to novel trisubstituted cyclic thickeners or
       gelators. Thus, cis, cis-1,3,5-cyclohexanetricarboxylic acid and
      \alpha-amino-N-6-quinolinylbenzenepropanamide dihydrobromide were reacted
       in the presence of triethylamine, 5.73 mmol of the resulting compound was
       reacted with 9.49 mmol 2-(2-hydroxyethoxy)ethylamine to give
      N, N'-bis [2-(2-hydroxyethoxy) ethyl] -N''-[(1S)-2-oxo-1-(phenylmethyl)-2-(6-
      quinolinylamino)ethyl]-1,3,5-cyclohexanetricarboxamide, showing gelation
       in water.
```

IT 613243-99-5P

RL: CPS (Chemical process); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of nonsym. gelling agents useful for pharmaceuticals, cosmetics, chromatog. materials, and catalytically active materials) 613243-99-5 HCAPLUS

RN 613243-99-5 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-, ( $1\alpha,3\alpha,5\alpha$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 800373-95-9P

RL: CPS (Chemical process); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of nonsym. gelling agents useful for pharmaceuticals, cosmetics, chromatog. materials, and catalytically active materials) 800373-95-9 HCAPLUS

RN 800373-95-9 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''[(1S)-2-oxo-1-(phenylmethyl)-2-(6-quinolinylamino)ethyl]-,
(1α,3α,5α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 800373-96-0P 852331-87-4P 852331-89-6P 852331-90-9P 852331-91-0P 852331-94-3P

852332-01-5P 852332-06-0P 852332-08-2P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of nonsym. gelling agents useful for pharmaceuticals, cosmetics, chromatog. materials, and catalytically active materials) 800373-96-0 HCAPLUS

RN 800373-96-0 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''[(1S)-2-oxo-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-,
(1α,3α,5α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852331-87-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[2-(2-naphthalenylamino)-2-oxo-1-(phenylmethyl)ethyl]-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852331-89-6 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[3-(methylthio)-1-[(2-naphthalenylamino)carbonyl]propyl]-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852331-90-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis(2-hydroxyethyl)-N''-[3-(methylthio)-1-[(2-naphthalenylamino)carbonyl]propyl]-, (1R,3S)- (9CI)

## (CA INDEX NAME)

Absolute stereochemistry.

RN 852331-91-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N-[3-(methylthio)-1-[(2-naphthalenylamino)carbonyl]propyl]-N',N''-bis(4-pyridinylmethyl)-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852331-94-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[2-[(4-methoxyphenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852332-01-5 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N-[2-(decylamino)-2-oxo-1-(phenylmethyl)ethyl]-N',N''-bis[2-(2-hydroxyethoxy)ethyl]-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852332-06-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[1-[(4-hydroxyphenyl)methyl]-2-(2-naphthalenylamino)-2-oxoethyl]-, (1R,3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 852332-08-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[2-oxo-2-[(2-phenylethyl)amino]-1-(phenylmethyl)ethyl]-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1036885 HCAPLUS

DOCUMENT NUMBER: 142:28161

TITLE: Production of small particles by thickening or

gelation

INVENTOR(S): Friggeri, Arianna; Van Bommel, Kjeld Jacobus Cornelis;

Robillard, George Thomas

PATENT ASSIGNEE(S): Applied Nanosystems B.V., Neth.

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PA'	TENT	NO.			KIN	<b>D</b> 1	DATE		Ž	APPL	ICAT	ION I	NO.		D.	ATE	
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	2003 W:	0975; 0975; AE, CO, GM, LS, PH, TZ,	B7 AG, CR, HR, LT, PL, UA, GM,	AL, CU, HU, LU, PT, UG, KE,	A3 AM, CZ, ID, LV, RO, US, LS,	AT, DE, IL, MA, RU, UZ, MW,	2004 AU, DK, IN, MD, SC, VC, MZ,	O311 AZ, DM, IS, MG, SD, VN, SD,	BA, DZ, JP, MK, SE, YU, SL,	BB, EC, KE, MN, SG, ZA, SZ,	BG, EE, KG, MW, SK, ZM, TZ,	BR, ES, KP, MX, SL, ZW UG,	BY, FI, KR, MZ, TJ,	BZ, GB, KZ, NI, TM,	CA, GD, LC, NO, TN,	CH, GE, LK, NZ, TR,	CN, GH, LR, OM, TT,
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	2003 W:	09755 09755 AE, CO, GM, LS, PH, TZ, GH, KG,	B7 AG, CR, HR, LT, PL, UA, GM,	AL, CU, HU, LU, PT, UG, KE, MD,	A3 AM, CZ, ID, LV, RO, US, RU, GR,	AT, DE, IL, MA, RU, UZ, MW, TJ,	2004 AU, DK, IN, MD, SC, VC, MZ, TM, IE,	AZ, DM, IS, MG, SD, VN, SD, AT, IT,	BA, DZ, JP, MK, SE, YU, SL, BE, LU,	BB, EC, KE, MN, SG, ZA, SZ, BG, MC,	BG, EE, KG, MW, SK, ZM, TZ, CH,	BR, ES, KP, MX, SL, ZW UG, CY, PT,	BY, FI, KR, MZ, TJ, ZM, CZ,	BZ, GB, KZ, NI, TM, ZW, DE, SE,	CA, GD, LC, NO, TN,	CH, GE, LK, NZ, TR, AZ, EE, SK,	CN, GH, LR, OM, TT, BY, ES, TR,

PRIORITY APPLN. INFO.:

WO 2003-NL381 A 20030522 EP 2003-78600 A 20031112 EP 2002-77007 A 20020522

OTHER SOURCE(S): MARPAT 142:28161

The present invention relates to a method for producing small particles of AB biol. and pharmaceutically active compds. A method for producing particles comprises (i) providing a solution of the compound of interest in a solvent, and (ii) inducing thickening or gelation of the solution using a thickener or gelator to produce particles by precipitation, freeze-drying, spray-drying or centrifuging. For example, to 12.5 mg of cHexAm(PheAmBn)(CH2CH2OCH2CH2OH)2 gelator (preparation given) and 1 mg of cyclosporin A (CyA), 50 µL of propylene glycol, 50 µL PEG 400 and 900  $\mu L$  water were added. The sample was heated till complete dissoln. of both the gelator and CyA was achieved and was then allowed to cool and thus gelate. TEM anal. of the gel shows the presence of gel fibers and CyA particles of average particle size of 40 to 100 nm. The bioavailability in rats of CyA obtained with the use of a gel was compared to that from the same formulation without gelator. When the CyA was administered in the gel formulation, CyA was recovered in the blood, with a maximal concentration

between 600 and 900 g/L after 4 to 6 h. In contrast, no detectable amts. of CyA were found in the blood when the CyA was administered in the ungelated form.

IT 613243-58-6P 697747-74-3P 800373-95-9P 800373-96-0P 800373-97-1P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (production of small particles by thickening or gelation)

RN 613243-58-6 HCAPLUS

CN L-Methionine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 697747-74-3 HCAPLUS

CN L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-, tris[2-(2-hydroxyethoxy)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 1-B

RN 800373-95-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''- [(1S)-2-oxo-1-(phenylmethyl)-2-(6-quinolinylamino)ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 800373-96-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''- [(1S)-2-oxo-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 800373-97-1 HCAPLUS

1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-CN [(1S)-2-[[(4-methoxyphenyl)methyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-,  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

--- OMe

L24 ANSWER 5 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:735309 HCAPLUS

141:325168 DOCUMENT NUMBER:

TITLE: Evaluation of chelating agents as anti-angiogenic

therapy through copper chelation

AUTHOR (S):

Camphausen, Kevin; Sproull, Mary; Tantama, Steve; Venditto, Vincent; Sankineni, Sandeep; Scott, Tamalee;

Brechbiel, Martin W.

CORPORATE SOURCE: Radioimmune & Inorganic Chemistry Section, Radiation

> Oncology Branch, National Cancer Institute, National Institutes of Health, Bethesda, MD, 20892-1002, USA

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(19),

5133-5140

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English OTHER SOURCE(S): CASREACT 141:325168

The evaluation of several sets of polyamine donor chelating agents including a selection of novel hexadentate 1,3,5-cis,cis-triaminocyclohexane (tach) based derivs. were performed in an in vitro endothelial cell proliferation assay to assess their cytotoxicity and selectivity as novel anti-angiogenic agents. The selective nature of the anti-angiogenic agents for human umbilical vein endothelial cells (HUVEC) was compared to a normal fibroblast cell line and a human Glioma cell line to evaluate these compds. Linear tri- and tetra-polyamines were superior to both macrocyclic and the tach based polyamine chelating agents in terms of selectivity of its inhibitory activity toward the proliferation of HUVEC cells compared to the fibroblast and human Glioma cells. The linear polyamine, triethylenetetramine, previously reported to possess anti-angiogenic properties failed to demonstrate any selectivity for inhibiting the proliferation of HUVEC cells compared to the fibroblast and human Glioma cells.

IT 769950-61-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(evaluation of polyamine chelating agents as anti-angiogenic therapy through copper chelation in relation to selective cytotoxicity towards vascular endothelial cells)

RN 769950-61-0 HCAPLUS

CN Carbamic acid,  $[(1\alpha, 3\alpha, 5\alpha) - 1, 3, 5 -$ 

cyclohexanetriyltris[imino(1,1-dimethyl-2-oxo-2,1-ethanediyl)]]tris-,
tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:344683 HCAPLUS

DOCUMENT NUMBER: 141:115894

TITLE: Nickel(II), copper(II) and zinc(II) binding properties

and cytotoxicity of tripodal, hexadentate tris(ethylenediamine)-analogue chelators

AUTHOR(S): Ye, Neng; Park, Gyungse; Przyborowska, Ann M.; Sloan, Paula E.; Clifford, Thomas; Bauer, Cary B.; Broker,

Grant A.; Rogers, Robin D.; Ma, Rong; Torti, Suzy V.;

Brechbiel, Martin W.; Planalp, Roy P.

CORPORATE SOURCE: Department of Chemistry, University of New Hampshire,

Durham, NH, 03824-3598, USA

SOURCE: Dalton Transactions (2004), (9), 1304-1311

CODEN: DTARAF; ISSN: 1477-9226

## Pryor 09 666463

PUBLISHER:

Royal Society of Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 141:115894

Three tripodal hexamine chelators based on cis,cis-1,3,5triaminocyclohexane (tach) were synthesized and their aqueous coordination
chemical with Ni(II), Cu(II) and Zn(II) is reported. The chelators have a
2-aminoethyl pendant arm attached to each nitrogen of tach, specifically
tachen' (N,N',N''-tris(2-aminoethyl)cyclohexane-cis,cis-1,3,5-triamine),
and two with S,S,S-chiral pendant arms, tachpn' (N,N',N''-tris(2aminopropyl)cyclohexane-cis,cis-1,3,5-triamine) and tachbn'
(N,N',N''-tris(2-amino-3-phenylpropyl)cyclohexane-cis,cis-1,3,5-triamine).

These chelators complex Ni(II), Cu(II) and Zn(II) in aqueous or

aqueous/methanolic

medium. The crystalline products [MIIL](X)2 are isolated, where M = Ni(II), Cu(II) or Zn(II), L = tachen, tachpn or tachbn, and X = ClO4-. Crystallog. study of selected tachpn and tachbn complexes shows the chelate arms are constrained in a  $\Lambda(\delta\delta\delta)$  configuration about M(II), which is attributed to their chirality. Solution UV-visible spectroscopy of the Ni(II) and Cu(II) complexes indicates six-coordination and little effect of the pendant arm substitution on ligand-field strength. The single exception is [Cu(tachbn)]2+, whose spectrum is consistent with five-coordination in solution The cytotoxicities of tachen, tachpn and tachbn toward cultured cancer cells is in the order tachen < tachpn < tachbn < tachpyr, where tachpyr is the aminopyridyl chelator N,N',N''-tris(2-pyridylmethyl)cyclohexane-cis,cis-1,3,5-triamine. The cytotoxicity difference is attributed to an order of increasing lipophilicity, tachen < tachpn < tachbn <

IT 717138-76-6P 717138-77-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate product in preparation of tris(aminoalkyl)cyclohexanetriamine chelating ligand)

RN 717138-76-6 HCAPLUS

CN Carbamic acid,  $[(1\alpha, 3\alpha, 5\alpha) - 1, 3, 5 -$ 

cyclohexanetriyltris[imino[(1S)-1-methyl-2-oxo-2,1-ethanediyl]]]tris-,
tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 717138-77-7 HCAPLUS

CN Carbamic acid,  $[(1\alpha, 3\alpha, 5\alpha)-1, 3, 5$ cyclohexanetriyltris[imino[(1S)-2-oxo-1-(phenylmethyl)-2,1ethanediyl]]]tris-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:290636 HCAPLUS

DOCUMENT NUMBER: 141:23890

TITLE: Responsive cyclohexane-based low-molecular-weight

hydrogelators with modular architecture

AUTHOR(S): van Bommel, Kjeld J. C.; van der Pol, Cornelia;

Muizebelt, Inouk; Friggeri, Arianna; Heeres, Andre;

Meetsma, Auke; Feringa, Ben L.; van Esch, Jan

CORPORATE SOURCE: BioMaDe Technology Foundation, Groningen, 9747 AG,

Neth.

SOURCE: Angewandte Chemie, International Edition (2004),

43(13), 1663-1667

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:23890

AB By using a cyclohexane-based scaffold to which various amino acid-based substituents can be connected, low-mol.-weight compds. were obtained that can gelate water at very low concns. Cis, cis-1,3,5-cyclohexanetricarbonyl amino acids and peptides were synthesized and shown to be excellent thermoreversible hydrogelators. The tyrosine analog grows good quality crystals; X-ray anal. shows that the mols. stack through the formation of a triple chain of intermol. hydrogen bonds of lengths ranging from 1.91 to 2.20 Å.

IT 697747-78-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of cyclohexanetricarbonyl tyrosine hydrogelator)

RN 697747-78-7 HCAPLUS

CN L-Tyrosine, N,N',N''-[( $1\alpha$ ,  $3\alpha$ ,  $5\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris-, hydrochloride, hydrate (2:2:3) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HO 
$$CO_2H$$
 O  $CO_2H$  OH  $CO_2H$ 

HCl

# ●3/2 H<sub>2</sub>O

Absolute stereochemistry. Rotation (-).

Absolute stereochemistry. Rotation (-).

RN 613243-64-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[2-(2-hydroxyethoxy)ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 613243-95-1 HCAPLUS

CN L-Histidine, 1,1',1''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris[L-methionyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 1-B

RN 613243-96-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-[[[2-(1H-imidazol-4-yl)ethyl]amino]carbonyl]-3-(methylthio)propyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 697747-74-3 HCAPLUS

CN L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-

cyclohexanetriyltricarbonyl]tris-, tris[2-(2-hydroxyethoxy)ethyl] ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-B

Relative stereochemistry.

Absolute stereochemistry.

IT 613243-56-4P 613243-61-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclohexanetricarbonyl amino acid or peptide hydrogelators)

RN 613243-56-4 HCAPLUS

CN L-Methionine, N, N', N''-  $[(1\alpha, 3\alpha, 5\alpha) - 1, 3, 5 -$ 

cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-61-1 HCAPLUS

CN L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## Pryor 09 666463

L24 ANSWER 8 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:189185 HCAPLUS

DOCUMENT NUMBER: 140:391426

TITLE: Highly potent and long-acting trimeric and tetrameric

inhibitors of influenza virus neuraminidase

AUTHOR(S): Watson, Keith G.; Cameron, Rachel; Fenton, Rob J.;

Gower, David; Hamilton, Stephanie; Jin, Betty; Krippner, Guy Y.; Luttick, Angela; McConnell, Darryl; MacDonald, Simon J. F.; Mason, Andy M.; Nguyen, Van;

Tucker, Simon P.; Wu, Wen-Yang

CORPORATE SOURCE: School of Chemistry, Biota Chemistry Laboratory,

Monash University, Victoria, 3800, Australia

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),

14(6), 1589-1592

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

AB A set of trimeric and tetrameric derivs. of the influenza virus neuraminidase inhibitor zanamivir have been synthesized by coupling a common monomeric zanamivir derivative onto various multimeric carboxylic acid core groups. These discrete multimeric compds. are all significantly more antiviral than zanamivir and also show outstanding long-lasting protective activity when tested in mouse influenza infectivity expts.

IT 686767-93-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and anti-influenza activity of trimeric and tetrameric derivs. of the influenza virus neuraminidase inhibitor zanamivir)

RN 686767-93-1 HCAPLUS

CN D-glycero-D-galacto-Non-2-enonic acid, 5-(acetylamino)-4[(aminoiminomethyl)amino]-2,6-anhydro-3,4,5-trideoxy-,
7,7',7''-[(1α,3α,5α)-1,3,5-cyclohexanetriyltris(carbonyl
imino-6,1-hexanediyl)]tris[carbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 12 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2005 ACS on STN L24 ANSWER 9 OF 60

2003:1011634 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 140:163833

Design, Synthesis, and in Vitro Biological Evaluation TITLE:

of Small Molecule Inhibitors of Estrogen Receptor

 $\alpha$  Coactivator Binding

Rodriguez, Alice L.; Tamrazi, Anobel; Collins, AUTHOR (S):

Margaret L.; Katzenellenbogen, John A.

CORPORATE SOURCE: Department of Chemistry, University of Illinois,

Urbana, IL, 61801, USA

Journal of Medicinal Chemistry (2004), 47(3), 600-611 SOURCE:

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB Nuclear receptors (NRs) complexed with agonist ligands activate transcription by recruiting coactivator protein complexes. In principle, one should be able to inhibit the transcriptional activity of the NRs by blocking this transcriptionally critical receptor-coactivator interaction directly, using an appropriately designed coactivator binding inhibitor (CBI). To guide our design of various classes of CBIs, we have used the crystal structure of an agonist-bound estrogen receptor (ER) ligand binding domain (LBD) complexed with a coactivator peptide containing the LXXLL signature motif bound to a hydrophobic groove on the surface of the LBD. One set of CBIs, based on an outside-in design approach, has various heterocyclic cores (triazenes, pyrimidines, trithianes, cyclohexanes) that mimic the tether sites of the three leucines on the peptide helix, onto which are appended leucine residue-like substituents. The other set, based on an inside-out approach, has a naphthalene core that mimics the two most deeply buried leucines, with substituents extending outward to mimic other features of the coactivator helical peptide. A fluorescence anisotropy-based coactivator competition assay was developed to measure the specific binding of these CBIs to the groove site on the ER-agonist complex with which coactivators interact; control ligand-binding assays assured that their interaction was not with the ligand binding pocket. The most effective CBIs were those from the pyrimidine family, the best

# Pryor 09\_666463

binding with Ki values of ca. 30  $\mu\text{M}.$  The trithiane- and cyclohexane-based CBIs appear to be poor structural mimics, because of equatorial vs. axial conformational constraints, and the triazene-based CBIs are also conformationally constrained by amine-substituent-to-ring resonance overlap, which is not the case with the higher affinity alkyl-substituted pyrimidines. The pyrimidine-based CBIs appear to be the first small mol. inhibitors of NR coactivator binding.

IT 656822-41-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and in vitro biol. evaluation of triazene-, pyrimidine-, trithiane-, cyclohexane-, and naphthalene-based small mol. inhibitors of estrogen receptor  $\alpha$  coactivator binding)

RN 656822-41-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-tris(2-methylpropyl)-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 10 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:1006725 HCAPLUS

DOCUMENT NUMBER: 140:64687

TITLE: Cosmetic compositions containing silicones and

organogelling agents

INVENTOR(S): Ferrari, Veronique; Mondet, Jean

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: PCT Int. Appl., 154 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
WO 2003105788	A2	20031224	20030602			
WO 2003105788	A3	20040401				
W: AE, AG, A	L, AM, AT	, AU, AZ, BA	, BB, BG, BR, BY,	BZ, CA, CH, CN,		
CO, CR, C	J, CZ, DE,	, DK, DM, DZ	, EC, EE, ES, FI,	GB, GD, GE, GH,		
GM, HR, H	J, ID, IL	, IN, IS, JP	, KE, KG, KP, KR,	KZ, LC, LK, LR,		
LS, LT, I	J, LV, MA,	, MD, MG, MK	, MN, MW, MX, MZ,	NO, NZ, OM, PH,		
PL, PT, I	, RU, SC	, SD, SE, SG	, SK, SL, TJ, TM,	TN, TR, TT, TZ,		
UA, UG, U	S, UZ, VC	, VN, YU, ZA	, ZM, ZW			
RW: GH, GM, I	E, LS, MW,	, MZ, SD, SL	, SZ, TZ, UG, ZM,	ZW, AM, AZ, BY,		
KG, KZ, M	, RU, TJ	, TM, AT, BE	, BG, CH, CY, CZ,	DE, DK, EE, ES,		

## Pryor 09\_666463

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             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                  20031219
     FR 2840807
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                                              FR 2002-7206
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                           A2
                                  20050323
                                              EP 2003-759973
                                                                       20030602
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     US 2004170586
                           A1
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PRIORITY APPLN. INFO.:
                                               FR 2002-7206
                                                                       20020612
                                              US 2002-391617P
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                                                                       20020627
                                              US 2002-166648
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                                              US 2002-166650
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                                                                    A2 20020612
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                                                                    A2 20021220
                                              US 2003-438770P
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                                                                       20030109
                                              US 2003-438782P
                                                                    Р
                                                                       20030109
                                              WO 2003-EP6463
                                                                    W
                                                                       20030602
                                              US 2003-617048
                                                                    A2 20030711
                                              US 2003-622689
                                                                    A2 20030721
OTHER SOURCE(S):
                          MARPAT 140:64687
     A cosmetic composition comprises a liquid fatty phase containing at least one
     silicone oil, structured with a gelling system. The gelling system
     comprises at least 1 polymer having a weight-average mol. weight of
500-500,000,
     containing at least 1 moiety comprising at least one polyorganosiloxane group
     and at least 2 groups capable of establishing hydrogen interactions, the
     polymer being solid at room temperature and soluble in the liquid fatty phase
at
     25-250°, and one non-polymeric organogelling agent. Thus, a
     lipstick contained DC-556 5, Parleam 5, hydrophobic treated pigments 10, a polyamide-silicone 15, preservative qs, N-laurylglutamic acid dibutylamide
     5, and cyclopentasiloxane gs to 100%.
IT
     189299-29-4 189299-30-7 189301-40-4
     212268-42-3 212268-43-4
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
        (cosmetic compns. containing silicones and organogelling agents)
RN
     189299-29-4 HCAPLUS
CN
     1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,
     (1\alpha, 3\alpha, 5\alpha) - (9CI) (CA INDEX NAME)
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Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 189299-30-7 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
 N  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me

RN 189301-40-4 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

-- CHMe2

212268-42-3 HCAPLUS RN

1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-1,3,5-trimethyl-, CN  $(1\alpha, 3\alpha, 5\beta)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

212268-43-4 HCAPLUS RN

1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-trioctadecyl-, CN  $(1\alpha, 3\alpha, 5\beta)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
 Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me

HCAPLUS COPYRIGHT 2005 ACS on STN L24 ANSWER 11 OF 60

2003:990958 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 140:47044

TITLE: Cosmetic make-up or sanitary composition, structured

by rigid form silicone polymers and organogelators

Ferrari, Veronique; Mondet, Jean L'oreal, Fr. INVENTOR(S):

PATENT ASSIGNEE(S):

Fr. Demande, 167 pp. SOURCE:

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 21

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2840807	A1	20031219	FR 2002-7206	20020612
FR 2840807	B1	20050311		
WO 2003105788	A2	20031224	WO 2003-EP6463	20030602
WO 2003105788	A3	20040401		

# Pryor 09\_666463

```
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1515684
                          A2
                                20050323
                                           EP 2003-759973
                                                                   20030602
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO.:
                                            FR 2002-7206
                                                                Α
                                                                   20020612
                                            US 2002-391617P
                                                                 Р
                                                                   20020627
                                            WO 2003-EP6463
                                                                W
                                                                   20030602
OTHER SOURCE(S):
                         MARPAT 140:47044
    A cosmetic make-up or sanitary composition comprises a liquid fatty phase
containing
     at least a silicone oil, structured by a gelling system having at least
     (1) a polymer of average mol. mass in weight from 500 to 500 000, comprising at
     least a polyorganosiloxane group made up from 1 to 1000 organosiloxane
     units in the chain or in the form of graft, and at least two groups able
     to establish hydrogen interactions, the polymer being solid at the ambient
     temperature and soluble in the fatty liquid phase at a temperature of
25-250°C, and
     at least (2) a not-polymeric organogelator. A lipstick contained
```

at least (2) a not-polymeric organogelator. A lipstick contained phenyltrimethicone (DC 556, 20 cSt) 5, hydrogenated isoparaffin (Parleam) 5, hydrophobic pigments (red iron oxide, yellow titanium oxide) 10, silicone polyamide 15, preservatives q.s., organogelator (N-laurylglutamic acid dibutylamide) 5, perfume q.s., and cyclopentasiloxane D5 q.s. 100%.

IT 189299-29-4 189299-30-7 189301-40-4 319922-90-2 319922-91-3

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (cosmetic make-up or sanitary composition, structured by rigid form silicone polymers and organogelators)

RN 189299-29-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
 Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me

RN 189301-40-4 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me<sub>2</sub>CH (CH<sub>2</sub>) 
$$\frac{Me}{3}$$
 Me (CH<sub>2</sub>)  $\frac{Me}{3}$  Me (CH<sub>2</sub>)  $\frac{Me}{3}$  Me  $\frac{Me}{4}$  (CH<sub>2</sub>)  $\frac{Me}{3}$  Me

PAGE 1-B

— CHMe₂

RN 319922-90-2 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 319922-91-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
N
H
 $(CH_2)_{17}$ 
N
H
 $(CH_2)_{17}$ 
Me

L24 ANSWER 12 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:929374 HCAPLUS

DOCUMENT NUMBER: 139:396167

TITLE: Preparation of amino acid derivatives as gelling

agents

INVENTOR(S): Van Bommel, Kjeld Jacobus Cornelis; Van Esch, Johannes

Henricus; De Loos, Maaike; Heeres, Andre; Feringa,

Bernard Lucas

PATENT ASSIGNEE(S): Applied Nanosystems B. V., Neth.

SOURCE: Eur. Pat. Appl., 17 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PAT	ENT I	NO.			KIN	D	DATE								D	ATE	
EP :	 1364	941			A1	~	2003	1126				7700			2	0020	522
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FΙ,	RO,	MK,	CY,	AL,	TR						
CA :	2486	675			AA		2003	1127		CA 2	003-	2486	575		2	0030	522
WO :	2003	0975	87		A2		2003	1127		WO 2	003-1	NL38	1		2	0030	522
WO :	2003	0975	37		<b>A</b> 3		2004	0311									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KΡ,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
							SC,						-		-		•
						-	VC,						•	•	•	•	•
	RW:				-	-	MZ,	-	-				ZM.	ZW.	AM.	AZ.	BY.
					-	•	TM,	•				•	•		•	•	•
							ΙE,										
EP :								GN, GQ, GW, ML, MR, NE, EP 2003-752951									
							ES,										
		-			-		RO,	-	-	-		•	•	•	•	•	~ - /
PRIORITY	APP			•	_ • ,	,	,	,	•	EP 2		•	•	•	•		522
INIONIII				• •						WO 2							
										2	005 1	. O C LL P.	_	,	. 2	0030.	J 4 4

OTHER SOURCE(S):

MARPAT 139:396167

The invention relates to a novel class of gelling agents Y1n-Am1-X1-Z(-X2-Am2-Y2n) (-X3-Am3-Y3n) [Z is (hetero)cycloalkyl or (hetero)aryl; X1, X2, X3 are NH, CO, or NHCO; Am1, Am2, Am3 are amino acids or derivs. or a number of amino acids or derivs.; Y1, Y2, Y3 are OH, OR, NHR, where R is (cyclo)alk(en)(yn)yl; n = 1 or 2 (with provisos)] and to a process for their preparation Thus, Z-[Phe-O(CH2)7CH:CH2]3 (Z is cis,cis-1,3,5-cyclohexanetricarbonyl) was prepared via amidation reaction and used to form a gel of Grubbs catalyst in benzene.

IT 627093-37-2 627093-38-3 627093-39-4

627093-41-8 627093-42-9

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (preparation of amino acid derivs. as gelling agents)

RN 627093-37-2 HCAPLUS

CN L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-, trioctyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 627093-38-3 HCAPLUS

CN L-Leucine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-, trioctyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 627093-39-4 HCAPLUS

CN L-Phenylalanine, N,N',N''-[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris-, tri-9-decenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

Ph

Ph

$$C(CH_2)_8$$
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 
 $C(CH_2)_8$ 

PAGE 1-B

 $\sim_{\text{CH}_2}$ 

RN 627093-41-8 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-2-(octylamino)-2-oxo-1-(phenylmethyl)ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me (CH<sub>2</sub>) 
$$7$$
  $\frac{H}{N}$   $\frac{H}{N}$ 

RN 627093-42-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-(octylamino)-2-oxoethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me (CH<sub>2</sub>) 
$$7$$
  $\frac{H}{N}$   $\frac{H}{N}$  (CH<sub>2</sub>)  $\frac{H}{7}$   $\frac{H}{N}$   $\frac$ 

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

13

L24 ANSWER 13 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2003:900772 HCAPLUS

DOCUMENT NUMBER: 141:146161

REFERENCE COUNT:

AUTHOR (S):

TITLE: Viscoelastic behavior of a supramolecular polymeric

system consisting of tri-3,7-dimethyloctyl

cis-1,3,5-cyclohexanetricarboxamide and n-decane Shikata, Toshiyuki; Oqata, Daisuke; Hanabusa, Kenji

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

CORPORATE SOURCE: Department of Macromolecular Science, Osaka

University, Osaka, 560-0043, Japan

SOURCE: Journal of the Society of Rheology, Japan (2003),

31(4), 229-236 CODEN: JSRJCZ

PUBLISHER: Society of Rheology, Japan

DOCUMENT TYPE: Journal LANGUAGE: English

The viscoelastic response of a supramol. organogel of tri-3,7dimethyloctyl-cis-1,3,5-cyclohexanetricarboxamide (DO3CH) and n-decane (C10) was examined varying the concentration of DO3CH (c) and temperature 20 -The storage modulus and loss modulus for the system were well described with the sum of two Maxwell models possessing two sets of a relaxation time and strength:  $\tau f$  and Gf, and  $\tau s$  (> $\tau f$ ) and Gs. By comparison, the viscoelastic response of organogels consisting of N,N',N''-tris(3,7-dimethyloctyl)benzene-1,3,5-tricarboxamide (DO3B) and n-alkanes is well described with only one Maxwell model. The value of Gf is proportional to c2 as observed in entangled flexible polymer systems and the organogels of DO3B. The value of Gs is approx. proportional to c1.3 similarly to that predicted for rigid rod-like polymer solns. The value of  $\tau f$  is essentially independent of c, while that of  $\tau s$  is kept at a constant and is followed by increasing above c = 10 g-L-1. The activation energy of relaxation times is less than that for the viscosity of C10. Supramol. polymeric structures bearing 2-type, rigid rod-like and flexible portions are generated in the system due to intermol. hydrogen bonding. The fast relaxation mode is attributed to the entanglement release between the flexible portions as observed in the organogels of DO3B, and slow relaxation is linked to rotational relaxation of the rigid rodlike portion.

#### IT 189301-40-4

RL: PRP (Properties)

(viscoelastic response of supramol. system of dimethyloctyl-cis-cyclohexanetricarboxamide and n-decane and adequacy of Maxwell model)

RN 189301-40-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,

 $(1\alpha, 3\alpha, 5\alpha)$  - [partial] - (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A Me Me Me<sub>2</sub>CH  $(CH_2)_3$  $(CH_2)_3$ N H

PAGE 1-B

--- CHMe2

CORPORATE SOURCE:

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 14 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

2003:851475 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 140:65724

TITLE: Orthogonal Self-Assembly of Low Molecular Weight

Hydrogelators and Surfactants

AUTHOR (S): Heeres, Andre; Van der Pol, Cornelia; Stuart, Marc;

> Friggeri, Arianna; Feringa, Ben L.; Van Esch, Jan BioMaDe Technology Foundation, Groningen, 9747, Neth.

SOURCE: Journal of the American Chemical Society (2003),

125 (47), 14252-14253 CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal English LANGUAGE:

The concurrent self-assembly of new 1,3,5-trisamide-cyclohexane-based low mol. weight hydrogelators and various surfactants in H2O gives self-assembled fibrillar networks with encapsulated micelles. This prototype system presents an example of orthogonal self-assembly, i.e., the independent formation of 2 different supramol. structures, each with their own characteristics that coexist within a single system.

IT 613243-58-6P 613243-59-7P 613243-64-4P

> RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(orthogonal self-assembly of low mol. weight hydrogelators and surfactants)

RN 613243-58-6 HCAPLUS

L-Methionine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)-1,3,5-$ CN

cyclohexanetriyltricarbonyl]tris- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 613243-59-7 HCAPLUS

CN L-Phenylalanine, N,N',N''-[( $1\alpha$ ,  $3\alpha$ ,  $5\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris-, tris(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-64-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[2-(2-hydroxyethoxy)ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

PAGE 1-B

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OH
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REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 15 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:818262 HCAPLUS

DOCUMENT NUMBER: 139:328317

TITLE: Delivery of a substance to a pre-determined site

INVENTOR(S): Friesen, Robert Heinz Edward; Leenhouts, Cornelis Johannes; Hektor, Harm Jan; Van Esch, Johannes

Henricus; Heeres, Andre; Robillard, George Thomas

PATENT ASSIGNEE(S): Applied Nanosystems B.V., Neth.

SOURCE: PCT Int. Appl., 303 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PA	PATENT NO.					KIND DATE			•	APPL	ICAT	ION	DATE					
WO	2003084508			A1 20031016				WO 2	003-1	NL25	20030404							
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NI,	NO,	NZ,	OM,	
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW						
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
·		KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	
		-					ΙE,	-	-	-	-	-	-	-				
		BF,	ΒJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
EP	1350	507			A1		2003	1008		EP 2	002-	7631	6		2	0020	404	
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR							
EP	1490	028			A1		2004	1229		EP 2	003-	7460	20030404					
	R:	•	-	•		-	ES,		-								PT,	
		•	-		LV,	FI,	RO,	MK,	-	-	•	•		•	•			
PRIORIT	Y APP	LN.	INFO	. :						EP 2								
															P 20020404			
										US 2						20020405		
	EP 2002-80481											0021						
							WO 2	003-1	NL25	6	Ī	N 2	0030	404				

OTHER SOURCE(S): MARPAT 139:328317

AB The invention is concerned with delivery vehicles for delivering a substance of interest to a predetd. site, said vehicle comprising said substance and a means for inducing availability of at least one compartment of said vehicle toward the exterior, thereby allowing access of said substance to the exterior of said vehicle at said predetd. site. The invention is further concerned with uses of said vehicle and methods for preparing it.

IT 613243-72-4 613243-75-7

#### Pryor 09 666463

RL: RCT (Reactant); RACT (Reactant or reagent) (delivery of a substance to a pre-determined site) RN613243-72-4 HCAPLUS Phenylalanine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris-, CN trimethyl ester (9CI) (CA INDEX NAME)

RN 613243-75-7 HCAPLUS

CN D-Phenylalanine, N-[[3-[[[(1S)-2-methoxy-1-[(4-nitrophenyl)methyl]-2oxoethyl]amino]carbonyl]-5-[[[(1S)-2-methoxy-2-oxo-1-(phenylmethyl)ethyl]amino]carbonyl]cyclohexyl]carbonyl]-4-nitro-, methyl ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 613243-56-4P 613243-57-5P 613243-58-6P 613243-59-7P 613243-60-0P 613243-61-1P 613243-62-2P 613243-63-3P 613243-64-4P 613243-68-8P 613243-69-9P 613243-71-3P 613243-73-5P 613243-74-6P 613243-76-8P 613243-78-0P 613243-79-1P 613243-81-5P 613243-82-6P 613243-87-1P 613243-94-0P 613243-95-1P 613243-96-2P 613243-99-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (delivery of a substance to a pre-determined site) RN 613243-56-4 HCAPLUS L-Methionine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)-1,3,5-$ CN

cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

RN 613243-57-5 HCAPLUS

CN Methionine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris-, trimethyl ester (9CI) (CA INDEX NAME)

RN 613243-58-6 HCAPLUS

CN L-Methionine, N,N',N''-[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 613243-59-7 HCAPLUS

CN L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)-1,3,5-$ cyclohexanetriyltricarbonyl]tris-, tris(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-60-0 HCAPLUS

CN L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-61-1 HCAPLUS

CN L-Phenylalanine, N,N',N''-[( $1\alpha$ ,  $3\alpha$ ,  $5\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-62-2 HCAPLUS

CN Glycine,  $1,1',1''-[(1\alpha,3\alpha,5\alpha)-1,3,5-$ 

cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)
Absolute stereochemistry. Rotation (-).

RN 613243-63-3 HCAPLUS

CN Glycine, 1,1',1''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-64-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[2-(2-hydroxyethoxy)ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 613243-68-8 HCAPLUS

CN L-Glutamic acid, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-, hexamethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-69-9 HCAPLUS

CN L-Aspartic acid, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris-, hexamethyl ester (9CI) (CA INDEX NAME)

RN 613243-73-5 HCAPLUS

CN D-Phenylalanine, N,N'-[[( $1\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-5-[[[((1S)-1-carboxy-2-phenylethyl]amino]carbonyl]-1,3-cyclohexanediyl]dicarbonyl]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-74-6 HCAPLUS

CN D-Phenylalanine, N-[[3-[[[(1S)-1-carboxy-2-(4-nitrophenyl)ethyl]amino]carbonyl]-5-[[[(1S)-1-carboxy-2-phenylethyl]amino]carbonyl]cyclohexyl]carbonyl]-4-nitro-, stereoisomer

### (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-76-8 HCAPLUS

CN D-Alanine, 1,1',1''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HO<sub>2</sub>C R N S N H O Me O Ph O Me 
$$HO_2$$
C R N S N H O Me

RN 613243-78-0 HCAPLUS

CN D-Alanine, 1,1',1''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, trimethyl ester (9CI) (CA INDEX NAME)

RN 613243-79-1 HCAPLUS

CN  $\beta$ -Alanine, 1,1',1''-[(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$HO_2C$$
 $HO_2C$ 
 $HO_2C$ 

RN 613243-81-5 HCAPLUS

CN  $\beta$ -Alanine, 1,1',1''-[(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

\_\_OMe

RN 613243-82-6 HCAPLUS

CN L-Glutamic acid, 1,1',1''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

# Pryor 09\_666463

PAGE 1-B

\_\_CO2H

RN 613243-87-1 HCAPLUS CN L-Glutamic acid, 1,1',1''-[(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, hexamethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 613243-94-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[3-(methylthio)-1-[[(4-pyridinylmethyl)amino]carbonyl]propyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 613243-95-1 HCAPLUS

CN L-Histidine, 1,1',1''-[ $(1\alpha,3\alpha,5\alpha)$ -1,3,5-cyclohexanetriyltricarbonyl]tris[L-methionyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-B

RN 613243-96-2 HCAPLUS

1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-[[[2-(1H-imidazol-4-CN yl)ethyl]amino]carbonyl]-3-(methylthio)propyl]-,  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN613243-99-5 HCAPLUS

1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethy1]-N''-[2-CN[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-,  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2005 ACS on STN L24 ANSWER 16 OF 60

ACCESSION NUMBER: 2003:561445 HCAPLUS

DOCUMENT NUMBER: 139:338257

TITLE: The chemistry of 2-alkenyl-5(4H)-oxazolones. IX.

Acid-catalyzed oligomerization

AUTHOR (S): Heilmann, Steven M.; Moren, Dean M.; Krepski, Larry

R.; Rasmussen, Jerald K.; Gaddam, Babu N.; Roscoe, Stephen B.; Lewandowski, Kevin M.; McIntosh, Lester H.; Roberts, Ralph R.; Fansler, Duane D.; Szekely,

### Pryor 09\_666463

Gabriella G.; Weil, David A.; Thakur, Khalid A.;
Pathre, Sadanand V.; Battiste, John L.; Hanggi,

Douglas A.

CORPORATE SOURCE: Organic Materials Technology Center, 3M, St. Paul, MN,

USA

SOURCE: Journal of Macromolecular Science, Pure and Applied

Chemistry (2003), A40(8), 755-790 CODEN: JSPCE6; ISSN: 1060-1325

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Results of the acid catalyzed oligomerization of 2-alkenyl-5(4H) - oxazolones are reported. Employing LC-MS and preparative LC methods, the oligomeric mixts. were characterized by NMR analyses and were discovered to consist of exclusively cyclic trimers to decamers, with tetramers and pentamers predominating. A nucleophilic oligomerization mechanism involving Michael addition and C-alkylation of a ketene-aminal to protonated monomer was proposed that resulted in irreversible cyclization at the trimer propagation stage. Subsequent oligomerization proceeded via enolization of  $\alpha$ -hydrogens on 2-substituted 5(4H)-oxazolone products and continued Michael addition to protonated monomer. In the sense that when both enolizable hydrogens and protonated monomer are present, the oligomerization can be regarded as being "living.".

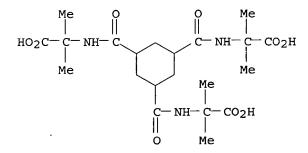
IT 616237-55-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(model compound; preparation of model compound for acid-catalyzed oligomerization of 2-alkenyl-5(4H)-oxazolones)

RN 616237-55-9 HCAPLUS

CN Alanine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris[2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 17 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:292147 HCAPLUS

DOCUMENT NUMBER: 139:52684

TITLE: Steric-factor-directed alternating supramolecular

copolymer composed of hydrogen-bonded

cyclohexanetricarboxamide units

AUTHOR(S): Takasawa, Ryoichi; Murota, Kazutoshi; Yoshikawa, Isao;

Araki, Koji

CORPORATE SOURCE: Institute of Industrial Science, University of Tokyo,

Tokyo, 153-8505, Japan

SOURCE: Macromolecular Rapid Communications (2003), 24(4),

335-339

### Pryor 09 666463

CODEN: MRCOE3; ISSN: 1022-1336

PUBLISHER:

Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Hydrogen-bonded supramol. pseudo-polymers were obtained by mixing cyclohexanetricarboxamides in chloroform solution The compds. are tris[3-(diisopropyloctylsilanyloxy)propyl]-cis,cis-1,3,5-cyclohexanetricarboxamide and tris[2-(diisopropyloctylsilanyloxy)-1-(diisopropyloctylsilanyloxymethyl)ethyl]-cis,cis-1,3,5-cyclohexanetricarboxamide. Upon evaporation of the solvent, the hydrogen-bonded supramol. assemblies formed fibrous structures. When the mixture was up to equimolarity, the supramol. pseudo-polymer was found to have an alternating sequence, attributed to steric effects of alkylsilyl groups.

IT 489468-25-9 489468-27-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(steric effects of substituents on alternating supramol.

hydrogen-bonded cyclohexanetricarboxamide pseudopolymer structure)

RN 489468-25-9 HCAPLUS

Relative stereochemistry.

Me 
$$(CH_2)_{7}$$
  $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{4}$   $(CH_2)_{5}$   $(CH_2)_{5}$ 

PAGE 1-B

RN 489468-27-1 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[bis(1-methylethyl)octylsilyl]oxy]-1-[[[bis(1-methylethyl)octylsilyl]oxy]methyl]e thyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 18 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:858259 HCAPLUS

DOCUMENT NUMBER: 138:122405

TITLE: Design, fabrication and properties of

triamidecyclohexane supramolecular fibers consisted of

hydrogen-bonded pseudo-polymer chains

AUTHOR(S): Takasawa, Ryoichi; Yoshikawa, Isao; Araki, Koji

CORPORATE SOURCE: Inst. of Industrial Science, Univ. of Tokyo, Tokyo,

153-8505, Japan

SOURCE: Kobunshi Ronbunshu (2002), 59(10), 616-622

CODEN: KBRBA3; ISSN: 0386-2186

PUBLISHER: Kobunshi Gakkai

DOCUMENT TYPE: Journal LANGUAGE: Japanese

AB Triamidecyclohexane derivs. were reported to form rigid pseudo-polymer chains by triple intermol. hydrogen bonds between their amide groups. The compound 2, tris[3-(diisopropyloctylsilyloxy)propyl]-cis,cis-1,3,5-cyclohexanetricarbox-amide, which was designed to cover its hydrogen-bonded pseudo-polymer chain by nonpolar flexible diisopropyloctylsilyl groups, was synthesized and fabricated into a

sufficiently flexible supramol. fiber by spinning at 150° (spinning rate was 8-11 m min-1). The IR spectra of the fiber confirmed formation of the pseudo-polymer chain by the triple intermol. hydrogen bonds between the amide groups, and the X-ray diffraction pattern showed high orientation of the pseudo-polymer chains along the fiber axis (orientation function fc = 0.6). Tensile strength of the fiber was around 1 MPa. Polarized microscopic observation indicated that the fiber did not have a uniformly oriented structure but was composed of domains in 10-50 mm scale, even after fabrication by spinning.

IT 189299-30-7P 489468-25-9P 489468-27-1P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(fiber; design, fabrication and properties of triamidecyclohexane supramol. fibers consisted of hydrogen-bonded pseudo-polymer chains)

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
  $(CH_2)_{17}$   $(CH_2)_{17}$ 

RN 489468-25-9 HCAPLUS

Me 
$$(CH_2)_{7}$$
  $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{3}$   $(CH_2)_{4}$   $(CH_2)_{5}$   $(CH_2)_{5}$ 

PAGE 1-B

$$-$$
Pr-i  
 $-$  (CH<sub>2</sub>) $\frac{}{7}$ Me

RN 489468-27-1 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[bis(1methylethyl)octylsilyl]oxy]-1-[[[bis(1-methylethyl)octylsilyl]oxy]methyl]e
thyl]-, (1α,3α,5α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

IT 489468-24-8P 489468-26-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; design, fabrication and properties of

triamidecyclohexane supramol. fibers consisted of hydrogen-bonded pseudo-polymer chains)

RN 489468-24-8 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3-hydroxypropyl)-,

 $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

HO 
$$(CH_2)_3$$
 N  $(CH_2)_3$  OH

RN 489468-26-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-hydroxy-1-(hydroxymethyl)ethyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L24 ANSWER 19 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:840287 HCAPLUS

DOCUMENT NUMBER: 138:182688

TITLE: Cyclotriveratrylene (CTV) as a new chiral triacid

scaffold capable of inducing triple helix formation of collagen peptides containing either a native sequence

or Pro-Hyp-Gly repeats

AUTHOR(S): Rump, Erik T.; Rijkers, Dirk T. S.; Hilbers, Hans W.;

de Groot, Philip G.; Liskamp, Rob M. J.

CORPORATE SOURCE: Department of Haematology, University Medical Center,

Utrecht, Neth.

SOURCE: Chemistry--A European Journal (2002), 8(20), 4613-4621

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:182688

AB A new triacid scaffold is described based on the cone-shaped cyclotriveratrylene (CTV) mol. that facilitates the triple helical folding of peptides containing either a unique blood platelet binding collagen sequence or collagen peptides composed of Pro-Hyp-Gly repeats. The latter

#### Pryor 09 666463

were synthesized by segment condensation using Fmoc-Pro-Hyp-Gly-OH. Peptides were coupled to this CTV scaffold and also coupled to the Kemp's triacid (KTA) scaffold. After assembly of peptide H-Gly-[Pro-Hyp-Gly]2-Phe-Hyp-Gly-Glu (OAll) -Arg-Gly-Val-Glu (OAll) -Gly-[Pro-Hyp-Gly]2-NH2 (13) by an orthogonal synthesis strategy to both triacid scaffolds, followed by deprotection of the allyl groups, the mol. constructs spontaneously folded into a triple helical structure. In contrast, the non-assembled peptides The melting temperature (Tm) of (+/-) CTV[CH2C-(O)N(H)Gly-[Pro-Hyp-Gly]2-Phe-Hyp-Gly-Glu-Arg-Gly-Val-Glu-Gly-[Pro-Hyp-Gly]2-NH2]3 (14) is 19°C, whereas KTA[Gly-Gly-[Pro-Hyp-Gly]2-Phe-Hyp-Gly-Glu-Arg-Gly-Val-Glu-Gly-[Pro-Hyp-Gly]2-NH2]3 (15) has a Tm of 20°C. was shown for the first time that scaffolds were also effective in stabilizing the triple helix of native collagen sequences. The different stabilizing properties of the two CTV enantiomers could be measured after coupling of racemic CTV triacid to the collagen peptide, and subsequent chromatog. separation of the diastereomers. After assembly of the two chiral CTV scaffolds to the model peptide H-Gly-Gly-(Pro-Hyp-Gly)5-NH2 (24), the (+) -enantiomer of CTV 28b was found to serve as a better triple helix-inducing scaffold than the (-)-enantiomer 28a. In addition to an effect of the chirality of the CTV scaffold, a certain degree of flexibility between the CTV cone and the folded peptide was also shown to be of importance. Restricting the flexibility from two to one glycine residues resulted in a significant difference between the two collagen mimics 20a and 20b, whereas the difference was only slight when two glycine residues were present between the CTV scaffold and the peptide sequence in collagen mimics 30a and 30b.

IT 183888-51-9

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(cyclotriveratrylene (CTV) as chiral triacid scaffold capable of inducing triple helix formation of collagen peptides containing either a native sequence or Pro-Hyp-Gly repeats)

RN 183888-51-9 HCAPLUS

CN Glycine, N,N',N''-[[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 20 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:838235 HCAPLUS

DOCUMENT NUMBER: 138:90066

TITLE: TREN (Tris(2-aminoethyl)amine): An Effective Scaffold

for the Assembly of Triple Helical Collagen Mimetic

Structures

#### Pryor 09 666463

AUTHOR(S): Kwak, Juliann; De Capua, Antonia; Locardi, Elsa;

Goodman, Murray

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of California, La Jolla, CA, 92093-0343, USA

SOURCE: Journal of the American Chemical Society (2002),

124(47), 14085-14091

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:90066

AB A new scaffold, TREN-(suc-OH)3 [TREN = tris(2-aminoethyl)amine, suc = succinic acid], was incorporated to assemble triple helixes composed of Gly-Nleu-Pro sequences (Nleu = N-isobutylglycine). Extensive biophys. studies, which included denaturation studies, CD and NMR spectroscopy, and mol. modeling demonstrated that TREN-[suc-(Gly-Nleu-Pro)n-NH2]3 (n = 5,6) form stable triple helical structures in solution A comparative anal. of TREN-assembled and KTA-assembled collagen mimetics, KTA-[Gly-(Gly-Nleu-Pro)n-NH2]3 (n = 3,6; KTA = 1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid), indicates that the flexibility of the TREN scaffold is superior to the KTA scaffold in inducing triple helicity. This effect most likely arises from the flexibility of the TREN scaffold which allows the three peptide chains to adjust their register for a tighter triple helical packing.

IT 191537-50-5

RL: PRP (Properties)

(comparisons of biophys. properties of other helical peptides as collagen mimetics)

RN 191537-50-5 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1\alpha,3\alpha,5\alpha)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycylN-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

# PAGE 1-B

PAGE 1-C

PAGE 2-A

THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS 60 REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 21 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:792417 HCAPLUS

DOCUMENT NUMBER:

137:318027

TITLE:

Liquid crystalline compositions having high order parameter, azo dyes for the compositions, and

guest-host type liquid crystal devices thereof

INVENTOR(S):

Okamura, Hisashi; Kato, Takashi Fuji Photo Film Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 35 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
JP 2002302674	A2	20021018	JP 2001-107254	20010405		
PRIORITY APPLN. INFO.:			JP 2001-107254	20010405		
OTHER SOURCE(S):	MARPAT	137:318027				

GΙ

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
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The liquid crystalline compns. contain compds. bearing a plurality of chromophores, ≥2 of which are linked in such a way that conjugate planes of the chromophores can align parallel to each other. The compds. may be Ia or Ia' [Da1, Da2, Da1', Da2' = substituent containing chromophores such as those of azo dyes; Ral-Ra6, Ral'-Ra6' = H, substituent; 2 of Ra1-Ra6, being bonded to adjacent C, may be bonded to each other and form ring; X, Y = O, S, NR1, (substituted) C; R1 = alkyl, H]. Azo compds. shown as IIa (Ra1-Ra16 = H, substituent; 2 of Ra1-Ra16 = same as Ra1-Ra6; La1, La2 = linkage; na1, na2 = 0, 1;  $\geq$ 1 of Ra7-Ra11and  $\geq$ 1 of Ra12-Ra16 are azo group-containing substituent) will be employed as Ia in the compns. Also claimed are liquid crystalline compns. containing compds. whose ≥3 chromophores, maybe those of azo dyes or anthraquinone dyes, are linked via dendritic residues. The compds. will be represented by the formula Xb[(Lb)nb1Db]nb (Xb = dendritic residue; Db = chromophore such as those of azo dyes or anthraquinone dyes; Lb = linkage; nb1 = 0, 1; nb = 3-256 integer). Also claimed are liquid crystalline compns. containing compds. whose ≥3 chromophores, maybe those of azo dyes or anthraquinone dyes, are linked via cyclic groups containing ≥3 atoms bonded to chromophores

≥3 chromophores, maybe those of azo dyes or anthraquinone dyes, are linked via cyclic groups containing ≥3 atoms bonded to chromophores directly or via linkages. The compds. will be represented by the formula Xc[(Lc)ncDc]nc1 [Xc = cyclic group capable to be bonded to (Lc)ncDc with number of nc1; Dc = chromophore such as those of azo dyes or anthraquinone dyes; nc = 0, 1; nc1 = 3-256 integer].

IT 472985-56-1P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(dichroic liquid crystalline compns. having high order parameter, azo dyes for

compns., and guest-host type LCD thereof)

RN 472985-56-1 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis [4-[4-[(1E)-(4-butylphenyl)azo]phenoxy]butyl]-N''-[[4-[(1E)-(4-butylphenyl)azo]phenoxy]methyl]-1,3,5-trimethyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

PAGE 1-A

n-Bu----

PAGE 1-B

PAGE 1-C

L24 ANSWER 22 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:465762 HCAPLUS

DOCUMENT NUMBER: 137:52019

TITLE: Cosmetic compositions structured with a polymer containing a heteroatom and an organogelator

INVENTOR(S): Ferrari, Veronique

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.									APPLICATION NO.						DATE				
WO	2002	0476	28		<b>A1</b>	20020620			1	WO 2	000-	IB20:	20001213							
	W:	ΑE,	AG,	ΑL,	AM,	ΑT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,			
		CR,	CU,	CZ,	DΕ,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,			
		HU,	ID,	IL,	IN,	IS,	JΡ,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,			
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,			
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	2002				A3		2002		WO 2001-IB2780					20011212						
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		•	•	•	AM,		•	•	•	•										
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	CH,			
		CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	ΝL,	PT,	SE,	TR,			
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NΕ,	SN,	TD,	TG			
EP	1294	342			A2	:	2003	0326	]	EP 2	001-	9880	98		2	0011	212			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,			
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	ΑĹ,	TR									
JP	2004	5178	56		<b>T</b> 2	:	2004	0617		JP 2	002-	5557	57		2	0011	212			
US	20042	2239	87		A1	:	2004	1111	1	US 2	002-	1293	77		2	0021	016			
PRIORIT	Y APP	LN.							1	WO 2	000-	IB20:	28	1	A 2	0001	213			
			-							WO 2						0011	212			
OTHER SOURCE(S):					MAR	PAT	137:	5201		_			-							

OTHER SOURCE(S): MARPAT 137:52019

AB A physiol. acceptable composition, in particular a cosmetic composition, comprising

at least one liquid fatty phase which comprises (i) at least one structuring polymer having a polymer skeleton which comprises at least one hydrocarbon-based repeating unit containing at least one hetero atom; and (ii) at least one organogelator. A polymer skeleton is chosen from polyurethane, polyurea, and polyurethane-polyurea skeletons, and at least one structuring polymer is chosen from polyamide polymers. For example, a lipstick was prepared containing: Phase A - Uniclear 100 18%, GP-1 5%. isononyl isononanoate 3.33%, diisostearyl malate 15.33%, and hydrogenated polybutene 2.34%; Phase B - hydrophobic silica 3%, hydrogenated polybutene 25%, and isononyl isononanoate 12%; Phase C - pigments 7% and hydrogenated

### Pryor 09\_666463

polybutene 9%. The sticks of lipstick obtained had a diameter of 12.7 mm and a hardness of  $204\pm20$  g measured using a "cheese wire". The sticks of lipstick did not break during measurement of the dynamic fragility carried out on 3 sticks.

IT 189299-29-4 189299-30-7 189301-40-4 212268-42-3 212268-43-4

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (anhydrous cosmetic compns. with liquid fatty phase containing structuring polymers and organogelators)

RN 189299-29-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $N$   $(CH_2)_{11}$   $N$   $(CH_2)_{11}$   $N$   $(CH_2)_{11}$   $N$   $(CH_2)_{11}$   $N$   $(CH_2)_{11}$   $N$   $(CH_2)_{11}$   $($ 

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$

Me  $(CH_2)_{17}$ 

Me  $(CH_2)_{17}$ 

Me  $(CH_2)_{17}$ 

Me

RN 189301-40-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Me<sub>2</sub>CH (CH<sub>2</sub>) 
$$\frac{Me}{3}$$
 Me (CH<sub>2</sub>)  $\frac{Me}{3}$  Me (CH<sub>2</sub>)  $\frac{Me}{3}$  Me

PAGE 1-B

∠CHMe<sub>2</sub>

RN 212268-42-3 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-1,3,5-trimethyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 212268-43-4 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Me 
$$(CH_2)_{17}$$
 Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me

### Pryor 09 666463

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 23 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:403904 HCAPLUS

DOCUMENT NUMBER: 136:406922

TITLE: Dental restorative composite

INVENTOR(S): Angeletakis, Christos PATENT ASSIGNEE(S): Kerr Corporation, USA

SOURCE: U.S., 15 pp., Cont.-in-part of U.S. 6,127,450.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 7

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6395803	B1	20020528	US 2000-567547	20000505
US 6127450	Α	20001003	US 1998-93778	19980609
BR 9901799	Α	20000509	BR 1999-1799	19990608
JP 2000143431	A2	20000523	JP 1999-161599	19990608
CN 1245678	A	20000301	CN 1999-108075	19990609
MX 9905338	Α	20001031	MX 1999-5338	19990609
US 6384106	B1	20020507	US 2000-562190	20000502
PRIORITY APPLN. INFO.:			US 1998-93778	A2 19980609

OTHER SOURCE(S): MARPAT 136:406922

The present invention provides a resin-based dental restorative that exhibits high condensability, low volumetric shrinkage and low shrinkage stress. One or more of a rheol. modifier, dispersant and fluoro copolymer are mixed with a methacrylate resin and a fine mineral filler in amts. effective to improve the condensability of the resulting composite to achieve amalgam-like condensation, to reduce the volumetric shrinkage during polymerization, to improve wear resistance, and to provide a composite with generally improved phys. properties. Thus, a resin formulation was prepared from bis-GMA 3.0, triethylene glycol dimethacrylate 24.7, ethoxylated bisphenol A dimethacrylate 71.1, camphorquinone 0.17, 2-hydroxy-4-methoxy benzophenone 0.49, and BHT 0.05% by weight This was mixed with a filler composition consisting of barium aluminum silicate (silanized) 91.4, hydrophobic fumed silica (TS-530) 4.3, and fumed silica (OX-50) 4.3% by weight The use of the rheol. modifier reduced the volume of shrinkage significantly.

IT 189299-29-4 189299-29-4D, alkyl derivs.

RL: MOA (Modifier or additive use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(dental restorative composite)

RN 189299-29-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN189299-29-4 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI)(CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2005 ACS on STN L24 ANSWER 24 OF 60

ACCESSION NUMBER:

2002:185110 HCAPLUS

DOCUMENT NUMBER:

136:247832

TITLE:

Preparation of sialic acid dendrimers as multivalent neuraminidase inhibitors and anti-influenza agents

INVENTOR(S):

Wu, Wen-Yang; Dowle, Michael Dennis; Jin, Betty; Macdonald, Simon John Fawcett; Mason, Andrew McMurtrie; McConnell, Darryl; Watson, Keith

Biota Scientific Management Pty. Ltd., Australia

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT 1	KIN	D :	DATE			APPLICATION NO.					DATE							
					-													
WO 2002020514				A1 20020314				WO 2001-AU1128							20010907			
W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
	GM,	HR,	ΗU,	ID,	ΙL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,		
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PH,	PL,		
	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	ŪĠ,		

# Pryor 09\_666463

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US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                               CA 2001-2416336
     CA 2416336
                           AA
                                  20020314
                                                                        20010907
                                               AU 2001-85601
     AU 2001085601
                           Α5
                                  20020322
                                                                        20010907
     EP 1315719
                           A1
                                  20030604
                                               EP 2001-964755
                                                                        20010907
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2001013755
                           Α
                                  20030708
                                               BR 2001-13755
                                                                        20010907
     JP 2004507564
                           T2
                                  20040311
                                               JP 2002-525135
                                                                        20010907
     US 2004058853
                           A1
                                  20040325
                                               US 2003-363988
                                                                        20031014
PRIORITY APPLN. INFO.:
                                               AU 2000-10
                                                                    A 20000908
                                                                  W 20010907
                                               WO 2001-AU1128
OTHER SOURCE(S):
                          MARPAT 136:247832
GI
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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to a dendrimer compds. I in which: X is O or CH; R2 is azido, hydroxy, guanidino, amino, amidine, imidate; R2 is acyl or sulfonyl; Y is O, substituted amine; CG is a core group selected from an optionally substituted cyclic, straight or branched group or a combination thereof having from 1 to 200 atoms in its backbone, in which the backbone atoms are selected from C, N, O and S; and L is a linking group of from 0 to 20 backbone atoms, in which the backbone and terminal atoms are selected from C, N, O and S; or a pharmaceutically acceptable salt or derivative thereof which comprises three or more neuraminidase-binding groups attached to a spacer or linking group, in which the neuraminidase-binding group is a compound which binds to the active site of influenza virus neuraminidase, but is not cleaved by the neuraminidase. The invention also relates to processes for the preparation of the multimeric compound defined

above, pharmaceutical compns. containing them or methods for the treatment and/or prophylaxis of a viral infection involving them. Thus, dendrimer II.3CF3CO2H salt [R1 = guanidino, R2 = acetyl, Y = 0, L = CON(CH2)6] was prepared and tested in mice as neuraminidase inhibitor and anti-influenza agent (dose = 0.01-1 mg/kg).

IT 403660-73-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of sialic acid dendrimers as multivalent neuraminidase inhibitors and antiinfluenza agents)

RN 403660-73-1 HCAPLUS

CN D-glycero-D-galacto-Non-2-enonic acid, 5-(acetylamino)-4[(aminoiminomethyl)amino]-2,6-anhydro-3,4,5-trideoxy-,
7,7',7''-[1,3,5-cyclohexanetriyltris(carbonylimino-6,1hexanediyl)]tris[carbamate] (9CI) (CA INDEX NAME)

#### PAGE 1-A

#### PAGE 1-B

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 25 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:225289 HCAPLUS

DOCUMENT NUMBER: 134:256618

TITLE: Cosmetic composition containing a cyclohexane

derivative

INVENTOR(S): Livoreil, Aude PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

### Pryor 09\_666463

PATENT NO.						D	DATE			APPLICATION NO.						DATE			
EP	EP 1086945			A1 200			0010328			2000	-4023	20000828							
EP	1086	945			В1		2002	1009											
	R:	ΑT,	BE,	CH,	DE,	DK	, ES,	FR,	GB,	GF	R, IT	, LI,	LU,	NL,	SE,	MC,	PT,		
		ΙE,	SI,	LT,	LV,	FI	, RO												
FR	2798	655			<b>A1</b>		2001	0323		FR	1999	-1177	3		1	9990	921		
FR	2798	655			В1		2001	1116											
AT	2257	66			E		2002	1015		AΤ	2000	-4023	69		2	0000	828		
ES	2184	686			Т3		2003	0416		ES	2000	-4023	69		2	0000	828		
JP	2001	1146	30		A2		2001	0424		JP	2000	-2877	97		2	0000	921		
PRIORIT	Y APP	LN.	INFO	. :						FR	1999	-1177	3		A 1	9990	921		
OTHER S	OURCE	(S):			MARI	PAT	134:	2566	18										
CT																			

Ι

AΒ A cosmetic composition containing a cyclohexane derivative [I; R = H, saturated hydrocarbon; Y = COSR', CONHR', NHCOR', SCOR' (R' = H, an aryl group substituted with a hydrocarbon chain)]. Thus, cis-1,3,5tris(oleylaminocarbonyl)cyclohexane (II) was prepared by the reaction of cis 1,3,5-cyclohexane-tricarboxylic acid with oleylamine. A cosmetic stick contained II 20.8, iron oxide 0.5 g, isododecane 16, and parleam oil 4 mL. 330974-81-7 330974-82-8 330974-83-9 IT330974-84-0 330974-85-1 330974-86-2 330974-87-3 330974-88-4 330974-89-5 330974-90-8 330974-91-9 330974-92-0 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (cosmetic composition containing cyclohexane derivative) 330974-81-7 HCAPLUS RN1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(1-oxohexadecyl)-, CN  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me (CH<sub>2</sub>) 
$$_{14}$$
 N H (CH<sub>2</sub>)  $_{14}$  N H (CH<sub>2</sub>)  $_{14}$  N H

RN 330974-82-8 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(1-oxododecyl)-,

 $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me (CH<sub>2</sub>) 
$$10$$
  $\frac{N}{H}$   $\frac{N}{H}$  (CH<sub>2</sub>)  $10$   $\frac{N}{H}$ 

RN 330974-83-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-eicosenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 
$$\frac{1}{9}$$
  $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{H}$   $\frac{1}{H}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$ 

PAGE 1-B

RN 330974-84-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9E)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

# Pryor 09\_666463

PAGE 1-A

Me 
$$(CH_2)_7$$
  $E$   $(CH_2)_7$   $N$   $H$   $(CH_2)_7$   $N$   $(CH_2)_7$   $N$ 

PAGE 1-B

RN 330974-85-1 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[(9Z)-1-oxo-9-octadecenyl]-N''-(1-oxooctadecyl)-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 
$$\frac{1}{7}$$
  $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$ 

PAGE 1-B

RN 330974-86-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N-(1-oxododecyl)-N',N''-bis[(9Z)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

### Pryor 09 666463

Me (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{H}$   $\frac{1}{S}$   $\frac{1}{R}$   $\frac{1}{H}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$ 

PAGE 1-B

$$\sim$$
 (CH<sub>2</sub>) $^{\prime}_{7}$  Me

RN 330974-87-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N-(3,7-dimethyl-1-oxooctyl)-N',N''-bis[(9Z)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$   $\frac{1}{Z}$ 

PAGE 1-B

$$\sim$$
 (CH<sub>2</sub>) $_{7}^{\text{Me}}$ 

RN 330974-88-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N-[(9Z)-1-oxo-9-octadecenyl]-N',N''-bis(1-oxooctadecyl)-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Me (CH<sub>2</sub>) 
$$\frac{16}{16}$$
  $\frac{N}{H}$   $\frac{N}{H}$  (CH<sub>2</sub>)  $\frac{7}{7}$   $\frac{Z}{Z}$  (CH<sub>2</sub>)  $\frac{N}{7}$  Me

RN 330974-89-5 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis(1-oxododecyl)-N''-[(9Z)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 
$$10$$
 N H CH<sub>2</sub>)  $10$  N H CH<sub>2</sub>  $10$  N H CH<sub>2</sub>

RN 330974-90-8 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis(3,7-dimethyl-1-oxooctyl)-N''- [(9Z)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me<sub>2</sub>CH (CH<sub>2</sub>)  $\frac{Me}{3}$  Me  $\frac{N}{H}$  (CH<sub>2</sub>)  $\frac{N}{7}$   $\frac{R}{Z}$ 

PAGE 1-B

RN 330974-91-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 
$$\frac{1}{7}$$
  $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$ 

PAGE 1-B

$$\sim$$
 (CH<sub>2</sub>) $\frac{}{7}$  Me

RN 330974-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-eicosenyl]-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>)  $\frac{1}{9}$   $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{H}$   $\frac{1}{H}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$ 

PATENT	NO.	KIND	DATE	APPLICATION NO.	DATE
EP 106		A1 B1	20010117 20040818	EP 2000-401661	20000613
EP 106 R:	AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IT, LI, LU, NL,	SE, MC, PT,
FR 279		A1	20010119 20030516	FR 1999-9178	19990715
AT 273	685	B1 E	20040915	AT 2000-401661	20000613
ES 222 CA 231	4.538	T3 AA	20050401 20010115	ES 2000-401661 CA 2000-2314538	20000613 20000704
US 637 JP 200	2235) 1058915	B1 A2	20020416 20010306	US 2000-617131 JP 2000-216708	20000714 20000717
PRIORITY AP OTHER SOURC GI		MARPAT	134:10564	FR 1999-9178 A 7	19990715

AB Solid form cosmetic compns. comprising an oil and gelling agent I are disclosed. The compns. are in the form of translucent anhydrous stick which are non-transferable. A composition containing I [R = H, Y = CONHR' (R' = C12 alkyl)] 200 mg, and isododecane 5 mL was prepared A solid stick contained above composition 0.8, pigments (iron oxide) 0.5 g, isododecane 16, and parleam oil 4 mL.

IT 189299-29-4 189299-30-7 189301-40-4 319922-90-2 319922-91-3

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(solid form cosmetic compns. comprising oil and specific gelling agent)

RN 189299-29-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,

PAGE 1-B

(CH<sub>2</sub>) 9 Me

IT 330974-79-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cosmetic composition containing cyclohexane derivative)

RN 330974-79-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-octadecenyl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$  (CH<sub>2</sub>)  $\frac{1}{7}$   $\frac{1}{Z}$ 

PAGE 1-B

 $\sim$  (CH<sub>2</sub>) $_{7}^{\sim}$  Me

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 26 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:45914 HCAPLUS

DOCUMENT NUMBER: 134:105647

TITLE: Solid form cosmetic compositions comprising an oil and

a specific gelling agent

INVENTOR(S): Livoreil, Aude; Mougin, Nathalie

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

 $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 189301-40-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

-- CHMe2

RN 319922-90-2 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 319922-91-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
 Ne  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 27 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:690425 HCAPLUS

DOCUMENT NUMBER: 134:4731

TITLE: One-step coupling of tris(hydroxymethyl)aminomethane

to aliphatic and aromatic carboxylic acids

AUTHOR(S): Villanueva, Ignacio; Hernandez, Bernadette; Chang,

Virginia; Heagy, Michael D.

CORPORATE SOURCE: Department of Chemistry, New Mexico Institute of

Mining and Technology, Socorro, NM, 87801, USA

SOURCE: Synthesis (2000), (10), 1435-1438

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:4731

AB A convenient and general method was established to append tri-, hexa-, and nonadentate ligands about an aromatic or aliphatic core. This approach allows

variety of com. available carboxylates to be transformed to their N-[tris(hydroxymethyl)methyl]carboxamides in one step. The selective activation of the acid functionality to form the polyhydroxylated dendritic cores was achieved using the acyl transfer agent N-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline (EEDQ).

IT 308357-62-2P

а

### Pryor 09\_666463

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of aliphatic and aromatic carboxamides from
 tris(hydroxymethyl)aminomethane)

RN 308357-62-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-, (1α,3α,5α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 28 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:421213 HCAPLUS

DOCUMENT NUMBER:

133:59703

TITLE:

Association of compounds in carbon dioxide and the

gels and/or microcellular foams therefrom for

fracturing subterranean formations

INVENTOR(S): Beckman, Eric J.; Hamilton, Andrew D.; Huang, Zhihua; Carr, Andrew; Enick, Robert M.

PATENT ASSIGNEE(S): Yale University, USA

SOURCE: PCT Int. Appl., 101 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ENT	NO.		KIND DATE			1	APPLICATION NO.					DATE				
WO	2000	0359	98		A2 20000622		WO 1999-US29574					19991215					
WO	2000	0359	98		<b>A3</b>	:	2000	1019									
	W:	ΑE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
		CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,
		IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	ΜΆ,
		MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,
		SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VN,	ΥU,	ZA,	ZW,	AM,
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM								
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,
		DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
		CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG				
ORITY APPLN. INFO.:			1	US 1998-112188P			•	P 19981215									
									US 1999-166164P P 19991118								

AB The viscosity of supercrit. CO2 is increased by combining a compound having

### Pryor 09 666463

a CO2-philic functional group, such as a fluoroalkyl, siloxane or alkylene oxide group, and an aggregating functional group, such as an amide, urea, carboxylic acid, or thiourea group, which enables the compound to form a supramol. network in solution with supercrit. CO2. The compound is aggregated in solution to form a supramol. network such that the viscosity of the supercrit. CO2 with the supramol. network is greater than that of the starting supercrit. CO2. The gels are useful as fracturing fluids, solvents for paints and oils, in coatings or insulating materials, or as fillers (no data). A microcellular foam is prepared by combining a compound having a CO2-philic functional group and an aggregating functional group which enables the compound to form a supramol. network in solution with supercrit. CO2, then removing the CO2. The microcellular foams can also be used for low-d. structural parts, high-temperature insulation, separation media,

adsorbents, and catalyst supports (no data).

IT 277750-49-9P 277756-64-6P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(association of compds. in carbon dioxide and gels and/or microcellular foams therefrom for fracturing subterranean formations)

RN 277750-49-9 HCAPLUS

CN Glycine, N,N',N''-[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-cyclohexanetriyltricarbonyl]tris-, tris(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

F<sub>3</sub>C 
$$(CF_2)_7$$
  $O$   $N$   $H$   $O$   $N$   $H$   $O$ 

PAGE 1-B

RN 277756-64-6 HCAPLUS

CN L-Aspartic acid, N,N',N''-(1,3,5-cyclohexanetriyltrcarbonyl)tris-, hexakis(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

L24 ANSWER 29 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:251206 HCAPLUS

DOCUMENT NUMBER: 133:30681

TITLE: Preparation and catalytic enantioselective reactions

of C3-symmetric tris(oxazoline)s derived from Kemp's

triacid

AUTHOR(S): Chuang, Tsung-Hsun; Fang, Jim-Min; Bolm, Carsten

CORPORATE SOURCE: Department of Chemistry, National Taiwan University,

Taipei, 106, Taiwan

SOURCE: Synthetic Communications (2000), 30(9), 1627-1641

CODEN: SYNCAV; ISSN: 0039-7911

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:30681

GI

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB Kemp's triacid was elaborated to optically pure tris( $\beta$ -

hydroxylamide)s, e.g. I, and tris(oxazoline)s, e.g. II. The resulting C3-sym. compds. were used in diethylzinc addns. to benzaldehyde and allylic oxidns. of cyclopentene, based on Kharash reaction conditions, to give the corresponding products in good chemical yields and moderate enantioselectivities.

IT 273722-21-7P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (stereoselective preparation of C3-sym. tris(carboxamide)s and tris(oxazoline)s from Kemp's acid as chiral ligands in asym. addition and allylic oxidation reactions)

RN 273722-21-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-2-hydroxy-1-methylethyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 273722-22-8P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (stereoselective preparation of C3-sym. tris(carboxamide)s and tris(oxazoline)s from Kemp's acid as chiral ligands in asym. addition and allylic oxidation reactions)

RN 273722-22-8 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-(hydroxymethyl)-2methylpropyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 273722-20-6P 273722-23-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(stereoselective preparation of C3-sym. tris(carboxamide)s and

tris(oxazoline)s from Kemp's acid as chiral ligands in asym. addition and allylic oxidation reactions)

RN 273722-20-6 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1R)-2-hydroxy-1-phenylethyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 273722-23-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-(hydroxymethyl)-2,2-dimethylpropyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 30 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:705529 HCAPLUS

DOCUMENT NUMBER: 132:108275

TITLE: Thermodynamics of Formation of the Triple Helix from

Free Chains and from Template-Constrained Chains of

Collagen-like Monodisperse Poly(Gly-Pro-Hyp)

Structures

AUTHOR(S): Locardi, Elsa; Kwak, Juliann; Scheraga, Harold A.;

Goodman, Murray

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of California at San Diego, La Jolla, CA, 92093-0343,

USA

SOURCE: Journal of Physical Chemistry A (1999), 103(49),

10561-10566

CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Statistical thermodn. methods, developed for treating the  $\alpha\text{-helix-coil}$  transition, are applied herein to describe the formation of the triple helix from short free chains and short template-constrained chains of collagen-like monodisperse poly(tripeptides), using poly(Gly-Pro-Hyp) as the example. For such short chains, application of the one-helical-sequence approximation indicates that there is very little unwinding from the ends, so that an all-or-none model is adequate to treat this transition. From the dependence of the helix nucleation and propagation parameters on chain length, concentration, and temperature,

the thermodn. parameters for formation of the triple helix from both free chains and template-constrained monodisperse poly(Gly-Pro-Hyp) chains are similar, and also similar to those for free poly(Gly-Pro-Pro) chains.

IT 176839-96-6

RL: PRP (Properties)

(thermodn. of formation of the triple helix from free chains and from template-constrained chains of monodisperse poly(Gly-Pro-Hyp) structures)

RN 176839-96-6 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1\alpha,3\alpha,5\alpha)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B

PAGE 1-C

PAGE 2-B

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 31 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:559232 HCAPLUS

DOCUMENT NUMBER: 131:316063

TITLE: Supramolecular liquid-crystalline materials formed by

hydrogen-bonded assembly processes

AUTHOR(S): Kato, Takashi; Yasuda, Takayasu; Kanie, Kiyoshi;

Ihata, Osamu; Mizoshita, Norihiro; Hanabusa, Kenji;

Ukon, Masakatsu; Shimizu, Yo

CORPORATE SOURCE: Department of Chemistry and Biotechnology, School of

Engineering, The University of Tokyo, Tokyo, 113-8656,

Japan

SOURCE: Polymer Preprints (American Chemical Society, Division

of Polymer Chemistry) (1999), 40(2), 1104-1105

CODEN: ACPPAY; ISSN: 0032-3934

PUBLISHER: American Chemical Society, Division of Polymer

Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

AB Hydrogen-bonded mesogenic complexes are of 2 types: identical mols. and different mols. Dialkoxyphenyl moieties were incorporated into the glutamic acid unit of folic acid. These derivs. exhibit thermotropic mesomorphic properties due to the hydrogen-bonded tetramer formation. Hydrogen-bonded complexes of 2,6-bis(acylamino)pyridine and 4-alkoxybenzoic acid exhibit various liquid crystal phases. The formation of anisotropic composites of gelling agents and nematic, smectic and discotic liquid crystals with well-organized structures is described.

IT 189299-30-7
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)

(hydrogen-bonded assembly of gelling agents in triphenylene derivative discotic liquid crystal)

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
  $(CH_2)_{17}$   $(CH_2)_{17}$ 

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 32 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:444485 HCAPLUS

DOCUMENT NUMBER: 131:157896

TITLE: Synthesis of simple multivalent  $\beta$ -D-GalNAc-

 $(1\rightarrow 4)$ - $\beta$ -D-Gal oligomers as probes for

investigating the interactions of P. aeruginosa pili

with multivalent receptors

AUTHOR(S): Jiao, Hailong; Hindsgaul, Ole

CORPORATE SOURCE: Department of Chemistry, University of Alberta,

Edmonton, AB, T6G 2G2, Can.

SOURCE: Journal of Carbohydrate Chemistry (1999), 18(5),

499-513

CODEN: JCACDM; ISSN: 0732-8303

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Five multivalent β-D-GalNAc-(1→4)-β-D-Gal oligomers were selected and synthesized as probes for investigating the adhesin-receptor interactions of P. aeruginosa pill with multivalent receptors. They were synthesized by the amide coupling reactions of 8-(N-2-aminoethyl)carboxamidooctyl 4-O-(2-acetamido-2-deoxy-β-D-galactopyranosyl)-β-D-galactopyranoside (1) with EDTA dianhydride, EDTA, Kemp's triacid and adipic acid with EDC, DIC and DCC combined with HOBt as coupling reagents and by the reaction of per-O-acetylated 1 with 1,3,5-benzenetricarbonyl trichloride followed by de-O-acetylation. These resulting multivalent compds. contain flexible C9 spacer arms as linkers attached to either flexible hydrophilic moieties or rigid hydrophobic cores.

IT 236743-67-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of simple multivalent oligosaccharides as probes for investigating the interactions of P. aeruginosa pili with multivalent receptors)

RN 236743-67-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[9-[[4-0-[2-(acetylamino)-2-deoxy-β-D-galactopyranosyl]-β-D- galactopyranosyl]oxy]-1-oxononyl]amino]ethyl]-1,3,5-trimethyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

#### PAGE 1-A

### PAGE 1-B

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 33 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:427215 HCAPLUS

DOCUMENT NUMBER: 131:90194

TITLE: Photoelectric converters and photoelectrochemical

cells thereof

INVENTOR(S): Shirato, Kentaro; Yanagida, Shozo; Shirai, Hiroyoshi;

Hanabusa, Kenji

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11185836	A2	19990709	JP 1997-363503	19971216
PRIORITY APPLN. INFO.:			JP 1997-363503	19971216

AB The photoelec. converters have a conductive substrate, a layer of semiconductor particles containing adsorbed dye on the substrate, a gel electrolyte, and a counter electrode; where the gel electrolyte contains an electrolyte and a gelling agent having mol. weight ≤1000. The salts are selected from metal iodide, quaternary ammonium iodide, quaternary imidazolium iodide, quaternary pyridinium iodide, metal bromide, quaternary ammonium bromide, S compds., viologen dye, and hydroquinone-quinone.

IT 189299-30-7

RL: DEV (Device component use); USES (Uses)

(electrolyte gelling agents for photoelectrochem. cells with dye adsorbed semiconductor electrodes)

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,

 $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
N
H
 $(CH_2)_{17}$ 
Me
 $(CH_2)_{17}$ 
Me

L24 ANSWER 34 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:198807 HCAPLUS

DOCUMENT NUMBER: 131:29032

TITLE: Design, synthesis and conformations of novel triple

helical collagen mimetic structures

AUTHOR(S): Goodman, Murray; Kwak, Juliann

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of California, La Jolla, CA, 92093-0343, USA

SOURCE: Proceedings - Indian Academy of Sciences, Chemical

Sciences (1999), 111(1), 35-49 CODEN: PIAADM; ISSN: 0253-4134

PUBLISHER: Indian Academy of Sciences

DOCUMENT TYPE: Journal LANGUAGE: English

AB We have synthesized collagen-like monodisperse structures. A series of single chain Ac-(Gly-Pro-Hyp)n-NH2 where n = 1, 3, 5, 6, 9 and template-assembled KTA-[Gly-(Gly-Pro-Hyp)n-NH2]3 analogs (n = 1, 3, 5, 6), where KTA is the Kemp triacid (cis-1,3,5-trimethyl cyclohexane-1,3,5-tricarboxylic acid), were assessed for triple helicity by CD, thermal denaturation and NMR spectroscopy. The KTA-based template induces a significant gain in free energy and reduces the critical chain length for

### Pryor 09 666463

triple helix formation over the acyl terminated single chain structures. Our approach also includes the incorporation of the peptoid residue N-isobutylglycine into the design for novel collagen-like sequences. have synthesized and characterized acetylated single chain and template-assembled analogs composed of Gly-Pro-Nleu and Gly-Nleu-Pro sequences. The achiral trimeric unit Gly-Nleu-Nleu was included as a quest sequence in a host structure such as Ac-(Gly-Pro-Hyp)3-(Gly-Nleu-Nleu)3-(Gly-Pro-Hyp)3-NH2 which retains triple helicity. A series of guest-host collagen mimetics composed of Gly-Nleu-Pro sequences as the host were synthesized and assessed for triple helicity. Guest sequences include Gly-Nleu-Nleu and Gly-Nx-Pro units, where Nx is the guest peptoid residue with alkyl and aralkyl side chains. We have continued to investigate functionalized template motifs and sequence variations. are examining the effects of functionalization and sequence variation on triple helical stabilities and mol. properties in order to design novel collagen-based biomaterials.

IT 226562-17-0 226562-18-1 226562-22-7

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(design, synthesis and conformations of novel triple helical collagen mimetic structures)

RN 226562-17-0 HCAPLUS

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 226562-18-1 HCAPLUS

CN Glycinamide, 1,1',1''-[[( $1\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-(1-methylethyl)glycylglycyl-L-prolyl-N-(1-methylethyl)glycylglycyl-L-prolyl-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

# PAGE 1-B

O H N O

PAGE 1-C

RN 226562-22-7 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1α,3α,5α)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycyl-N-(1-methylethyl)glycyl-Lprolylglycyl-N-(1-methylethyl)glycyl-L-prolylglycyl-N-(1methylethyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# PAGE 1-A

## PAGE 1-B

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REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 35 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:717725 HCAPLUS

DOCUMENT NUMBER: 130:4357

TITLE: Synthesis of low molecular weight organogelators and

their physical gelation

AUTHOR(S): Hanabusa, Kenji; Shirai, Hirofusa

CORPORATE SOURCE: Department of Functional Polymer Science, Faculty of

Textile Science and Technology, Shinshu University,

Ueda, 386-8567, Japan

SOURCE: Kobunshi Ronbunshu (1998), 55(10), 585-594

CODEN: KBRBA3; ISSN: 0386-2186

PUBLISHER: Kobunshi Gakkai

DOCUMENT TYPE: Journal LANGUAGE: Japanese

of

AB This article describes the low mol. weight gelators which were reported since 1996. Alkylamides and alkylureas derived from trans-1,2-diaminocyclohexane are excellent organogelators which can gelate a wide variety of organic solvents, from protic polar solvents to aprotic non-polar ones. The results of gelation test of di-urea derivs. indicate that the intermol. hydrogen bonding between ureylene units is as very useful as the intermol. hydrogen bonding between amides for mol. design of gelators.

Tridodecyl-1,3,5-benzenetricarboxamide is found to act as thickener,

because the addition of the small amount of this compound causes a marked rise

viscosity of hydrocarbons and oils. On the other hand, trioctadecyl-cis-1,3,5-cyclohexanetricarboxamide, which is structurally related to tridodecyl-1,3,5-benzenetricarboxamide, can cause phys. gelation of hydrocarbons and oils. Bolaform amides derived from L-valine or L-isoleucine are excellent organogelators for a wide variety of organic solvents, although they contain neither an aromatic moiety nor a long methylene segment. The bolaform amides are expected to be smoothly-biodegradable organogelators. Besides the above gelators, this article deals with the following compds.; 4,4',4''-tris(stearoylamino)triphenylamine, an equimolar mixture of isocyanuric acid and triaminopyrimidine containing a cholesterol segment,  $\gamma$ -alkoxybutyrolactone, quaternary ammonium halide salts, p-toluenesulfonic

### Pryor 09\_666463

acid salt of L-leucine alkyl ester, fluoroalkylated oligomers, a 24-residue peptide, a biotin derivative, a cholic acid derivative, an N-alkylgluconamide derivative, and an L-isoleucine derivative

IT 189299-30-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of low mol. weight organogelators and their phys. gelation)

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
  $(CH_2)_{17}$   $(CH_2)_{17}$ 

L24 ANSWER 36 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:665873 HCAPLUS

DOCUMENT NUMBER: 129:330490

TITLE: Preparation of cyclohexanetricarboxamide derivatives

as thickening and/or gelation agents

INVENTOR(S):
Hanabusa, Kenji; Kawakai, Atsushi; Shirai, Hiroyoshi;

Iyanagi, Koichi

PATENT ASSIGNEE(S): Pola Chemical Industries, Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10273477	A2	19981013	JP 1997-344691	19971215
JP 3500289	B2	20040223		
PRIORITY APPLN. INFO.:			JP 1997-29790 A	19970129
OTHER SOURCE(S):	MARPAT	129:330490		
GI				

$$R^1$$
 $R^1$ 
 $R^1$ 
 $R^1$ 
 $R^1$ 
 $R^1$ 
 $R^1$ 
 $R^1$ 
 $R^1$ 

The title compds. (I; R = C4-20 linear or branched alkyl; R1 = H, C1-4 AΒ alkyl), which provide thickening and/or gelation or stabilization means for fluid organic compds. or compns. containing them, are prepared Thus, cis-1,3,5-cyclohexanetri(carboxylic acid) was dissolved in CHCl3, treated with SOCl2, stirred at room temperature for 1 h, and concentrated, and then condensed

with hexylamine in the presence of Et3N in CH2Cl2 under heating to give the title compound (II). II (3 mg) was added to 1 cm3 pyridine, heated to 100°, and cooled to give a gel.

IT 189299-28-3P 189299-29-4P 189299-30-7P

189301-40-4P 215231-39-3P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of cyclohexanetricarboxamide derivs. as thickening and/or gelation agents)

RN189299-28-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trihexyl-,  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_5$$
 N  $(CH_2)_5$  Me  $(CH_2)_5$  Me

189299-29-4 HCAPLUS RN

1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, CN  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Pryor 09\_666463

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 189299-30-7 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
 N  $(CH_2)_{17}$  Me  $(CH_2)_{17}$  Me

RN 189301-40-4 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

- CHMe<sub>2</sub>

### Pryor 09\_666463

RN 215231-39-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,8-dimethylnonyl)-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me<sub>2</sub>CH (CH<sub>2</sub>) 
$$\frac{Me}{H}$$
 (CH<sub>2</sub>)  $\frac{Me}{H}$  (CH

PAGE 1-B

-CHMe2

L24 ANSWER 37 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:512440 HCAPLUS

DOCUMENT NUMBER: 129:221032

TITLE: Cosmetic, pharmaceutical, or food compositions

containing cyclohexanetricarboxamides as thickening

agents

INVENTOR(S): Hide, Kenji; Kawaue, Atsushi; Shirai, Hirofusa;

Iyanagi, Koichi

PATENT ASSIGNEE(S): Pola Chemical Industries, Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10212213	A2	19980811	JP 1997-29602	19970129
JP 3501612	B2	20040302		
PRIORITY APPLN. INFO.:			JP 1997-29602	19970129
OTHER SOURCE(S):	MARPAT	129:221032		
GI				

AB Title compns. contain cyclohexanetricarboxamides I (R = C4-20 alkyl; R' = H, C1-4 alkyl) as thickening or gelation agents. The compns. are stable at high temperature (.apprx.40°). A foundation was prepared from glyceryl triisooctanate 10, jojoba oil 10, dimethicone 10, carnauba wax 10, cis-I (R = hexyl, R' = H) (preparation given) 1, mica 19, talc 10, TiO2 10, yellow iron oxide 5, red iron oxide 2, and nylon powder 13 parts.

IT 189299-28-3P 189299-29-4P 189299-30-7P 189301-40-4P 212268-42-3P 212268-43-4P

RL: BUU (Biological use, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cyclohexanetricarboxamides as thickening or gelation agents for cosmetics, pharmaceuticals, and foods)

RN 189299-28-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trihexyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_5$$
 N  $(CH_2)_5$  Me  $(CH_2)_5$  Me

RN 189299-29-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$   $(CH_2)_{11}$ 

RN 189299-30-7 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$

Me  $(CH_2)_{17}$ 

Me  $(CH_2)_{17}$ 

Me  $(CH_2)_{17}$ 

Me  $(CH_2)_{17}$ 

RN 189301-40-4 HCAPLUS CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me<sub>2</sub>CH (CH<sub>2</sub>) 
$$\frac{Me}{3}$$
 Me (CH<sub>2</sub>)  $\frac{Me}{3}$  Me  $\frac{Me}{4}$  (CH<sub>2</sub>)  $\frac{Me}{3}$  Me

PAGE 1-B

-- CHMe2

RN 212268-42-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-1,3,5-trimethyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 212268-43-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L24 ANSWER 38 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:496607 HCAPLUS

DOCUMENT NUMBER: 129:245455

TITLE: Incorporation of Achiral Peptoid-Based Trimeric

Sequences into Collagen Mimetics

AUTHOR(S): Jefferson, Elizabeth A.; Locardi, Elsa; Goodman,

Murray

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of California San Diego, La Jolla, CA, 92093-0343, USA

SOURCE: Journal of the American Chemical Society (1998),

120(30), 7420-7428

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB This report represents initial studies of collagen mimetics with achiral peptoid-based trimeric sequences. The incorporation of achiral units into collagen-like structures is of considerable interest for the structural simplification of collagen-like biomaterials. The achiral unit Gly-Nleu-Nleu (Nleu = N-isobutylglycine) was positioned between

### Pryor 09\_666463

Gly-Pro-Hyp trimeric repeats in collagen-like structures in order to examine the effect of an achiral block on triple helicity. A series of single chain structures, Ac-(Gly-Pro-Hyp)n-(Gly-Nleu-Nleu)n-(Gly-Pro-Hyp)n-NH2 (n = 1-3), and a template-assembled structure, KTA-[Gly-(Gly-Pro-Hyp)2-(Gly-Nleu-Nleu) 2-(Gly-Pro-Hyp) 2-NH2] 3 (KTA = cis,cis-1,3,5trimethylcyclohexane-1,3,5-tricarboxylic acid), were investigated. Biophys. studies were carried out in both H2O and ethylene qlycol (EG)/H2O (2:1, volume/volume) solvents, using CD and optical rotation measurements. Highly cooperative melting curves from optical rotation detns. were obtained for Ac-(Gly-Pro-Hyp)n-(Gly-Nleu-Nleu)n-(Gly-Pro-Hyp)n-NH2 (n = 2, and KTA-[Gly-(Gly-Pro-Hyp)2-(Gly-Nleu-Nleu)2-(Gly-Pro-Hyp)2-NH2]3, revealing that the achiral trimer can participate in triple helical structures. These results were also supported by CD spectroscopy. For the mols. Ac-(Gly-Pro-Hyp)3-(Gly-Nleu-Nleu)3-(Gly-Pro-Hyp)3-NH2 and KTA-[Gly-(Gly-Pro-Hyp)2-(Gly-Nleu-Nleu)2-(Gly-Pro-Hyp)2-NH2]3, the presence of collagen-like structures was also supported by 1H NMR spectroscopy in H2O. For each structure, a distinct set of resonances, obtained at low temperature, disappeared once a thermal denaturation temperature was

reached. Furthermore, the anal. of NOE cross-peaks established the close packing of Pro, Hyp, and Nleu. The spatial proximity of Pro and Nleu residues and of Hyp and Nleu residues belonging to different chains was confirmed by mol. modeling of triple helical Ac-(Gly-Pro-Hyp)3-(Gly-Nleu-Nleu) 3 - (Gly-Pro-Hyp) 3-NH2.

IT183888-51-9

> RL: RCT (Reactant); RACT (Reactant or reagent) (incorporation of achiral peptoid-based trimeric sequences into collagen mimetics)

RN183888-51-9 HCAPLUS

Glycine, N,N',N''-[ $(1\alpha,3\alpha,5\alpha)-1,3,5$ -trimethyl-1,3,5-CN cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$HO_2C$$
 $Me$ 
 $Me$ 
 $Me$ 
 $HO_2C$ 
 $Me$ 
 $Me$ 
 $HO_2C$ 
 $Me$ 
 $Me$ 
 $Me$ 
 $HO_2C$ 
 $Me$ 
 $HO_2$ 

THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 39 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2005 ACS on STN L24 ANSWER 39 OF 60

ACCESSION NUMBER: 1998:233900 HCAPLUS

DOCUMENT NUMBER: 129:149208

TITLE: The activated core approach to combinatorial chemistry: a selection of new core molecules

AUTHOR (S):

Pryor, Kent E.; Shipps, W., Jr.; Skyler, David A.;

Rebek, Julius, Jr.

CORPORATE SOURCE: Skaggs Institute for Chemical Biology and Department

of Chemistry, The Scripps Research Institute, La

Jolla, CA, 92037, USA

### Pryor 09\_666463

SOURCE:

Tetrahedron (1998), 54(16), 4107-4124

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 129:149208

Ι

III

Four new activated core mols. I-IV, suitable for use in solution-phase AB combinatorial organic chemical have been prepared These mols. represent an attempt to further explore shape-space and increase the structural diversity of prepared libraries, as well as to incorporate recognition elements in the cores to increase the chances for interaction with biol. targets. Demonstrations of deconvolution strategies used to simplify complex libraries and build individual mol. species based on the cores are also provided.

206647-41-8P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of activated core mols. for preparation of combinatorial libraries)

206647-41-8 HCAPLUS RN

L-Phenylalanine, N,N',N''-[ $(1\alpha,3\alpha,5\beta)$ -1,3,5-CN

cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 40 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:31317 HCAPLUS

DOCUMENT NUMBER: 128:102343

TITLE: Preparation and uses of saccharide-containing

dendrimers with a cyclohexane-polyol or inositol core.

INVENTOR(S): Wiessler, Manfred; Gschrey, Markus; Von der Lieth,

Willi; Mier, Walter

PATENT ASSIGNEE(S): Deutsches Krebsforschungszentrum Stiftung des

Offentlichen Rechts, Germany; Wiessler, Manfred; Gschrey, Markus; Von der Lieth, Willi; Mier, Walter

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 9748711	A1 19971224	WO 1997-DE1278	19970618
W: JP, US			
RW: AT, BE, CH,	DE, DK, ES, FI,	FR, GB, GR, IE, IT, I	LU, MC, NL, PT, SE
DE 19624705	A1 19980108	DE 1996-19624705	19960620
EP 906325	A1 19990407	EP 1997-931626	19970618
R: AT, BE, CH,	DE, DK, ES, FR,	GB, IT, LI, NL, SE	
JP 2000513342	T2 20001010	JP 1998-502095	19970618
US 6417339	B1 20020709	US 1999-202843	19990308
PRIORITY APPLN. INFO.:		DE 1996-19624705	A 19960620
		WO 1997-DE1278	W 19970618

OTHER SOURCE(S): CASREACT 128:102343

GI

$$\begin{array}{c}
R^{2} + CH_{2} + O \\
R^{3} + CH_{2} + O \\
6 & O + CH_{2} + R^{1} \\
O + CH_{2} + R^{6} \\
R^{4} + CH_{2} + O \\
6 & O + CH_{2} + R^{5}
\end{array}$$

The invention relates to dendrimers comprising an initiator core with at least two functional groups and at least two saccharides. It also relates to the use thereof for various purposes e.g. as a catalyst in enantioselective synthesis, as a cellular adhesion inhibitor, as a carrier for medicinal agents or for purification of glycoproteins by affinity chromatog. Thus, 1,3,4,5,6-penta-O-benzyl-myo-inositol was reacted with 1,6-dibromo-hexane, followed by deprotection and azidation, and coupled with 6-bromo-hexyl-2,3,4,6-tetra-O-benzyl- $\beta$ -D-glucopyranoside, to give [(I); R1 = N3; R2-R6 = 2,3,4,6-tetra-O-benzyl- $\beta$ -D-glucopyranoside]. Using I as a column-chromatog. packing, racemic thalidomide was resolved.

IT 200201-40-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and uses of saccharide containing dendrimers with a cyclohexane-polyol or inositol core)

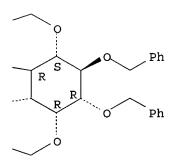
RN 200201-40-7 HCAPLUS

CN myo-Inositol,  $3,3',3''-0-[[(1\alpha,3\alpha,5\alpha)-1,3,5-$ cyclohexanetriyl]tris(carbonylimino-6,1-hexanediyl)]bis[1,2,4,5,6-pentakis-0-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### PAGE 1-A

### PAGE 1-B



L24 ANSWER 41 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:457086 HCAPLUS

DOCUMENT NUMBER: 127:81794

TITLE: Preparation of collagen-like peptoid

residue-containing triple helical structures

INVENTOR(S): Goodman, Murray; Taulane, Joseph P.; Feng, Yangbo;

Melacini, Giuseppe

PATENT ASSIGNEE(S): Regents of the University of California, USA

SOURCE: PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

									APPLICATION NO.									
									WO 1996-US18521									
	9719106																	
							BA,			BR	≀, B	ΒY,	CA,	CH,	CN,	CU,	CZ,	DE,
		DK,	EE,	ES,	FI,	GB,	GE,	HU,	IL,	IS	s, J	P,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK	C, M	IN,	MW,	MX,	NO,	ΝZ,	PL,	PT,
		RO,	RU,	SD,	SE,	SG,	SI,	SK,	TJ,	TM	1, T	R,	TT,	UA,	UG,	UΖ,	VN,	AM,
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM									
	RW:	ΚE,	LS,	MW,	SD,	SZ,	υG,	AT,	ΒĒ,	CH	I, D	Έ,	DK,	ES,	FI,	FR,	GB,	GR,
		ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	BJ	T, C	F,	CG,	CI,	CM,	GΑ,	GN,	ML,
		MR,	NE,	SN,	TD,	TG												
US	6096710				A 20000801				US 1996-668380						19960621			
CA	2237845				AΑ	AA 19970529			CA 1996-2237845						19961118			
AU								AU 1997-10549							19961118			
AU	716531				B2 20000224													
EP	861264			A2 1998090			0902	EP 1996-941391						19961118				
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	₹, I	Τ,	LI,	LU,	NL,	SE,	MC,	PT,
			FI															
	0. 2000000.							JP 1997-519839							19961118			
US	US 6329506				В1	20011211			US 1999-388916						19990901			
AU 750744				B2		2002	0725		AU	199	9-6	6531	7		1	9991	217	
AU	9965	317			A1		2000	0302										
PRIORITY APPLN. INFO.:									US	199	95 - (	6894	P		P 1	9951	117	
																	9960	
										WO	199	6-T	JS18	521		W 1	9961	118
OTHER SOURCE(S):				MAR	TAG	127:	81794	1										

AB Synthetic collagen derivs. in triple helical conformation and comprising amino acid chains of repeating trimers Gly-Xp-Pro, Gly-Pro-Yp, Gly-Pro-Hyp, and Gly-Pro-Pro [Xp, Yp = N-substituted glycine (peptoid) residue] of highly populated collagen sequences are claimed. The invention includes methods of preparing synthetic collagen structures having the triple helix conformation present in collagen from collagen-type polypeptides and poly(peptide-peptoid residue) chains by means of a helix-inducing template such as cis,cis-1,3,5-trimethyl-1,3,5-cyclohexanetricarboxylic acid (Kemp's triacid) and 1,3,5-benzenetricarboxylic acid. Thus, tripeptide sequence Boc-Gly-Pro-Hyp(CH2Ph)-MBHA resin was prepared, deprotected with 30% CF3CO2H in CH2Cl2, and coupled with Kemp triacid derivative I (R = OH) in the presence of HOBt and diisopropylcarbodiimide, followed by resin cleavage and deprotection to give 56% collagen-like structure I (R = Gly-Pro-Hyp-NH2).

IT 183888-50-8P 183888-51-9P 191537-47-0P
191537-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of collagen-like peptoid residue-containing triple helical structures)

RN 183888-50-8 HCAPLUS

CN Glycine, N,N',N''-[[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris-, tris(phenylmethyl) ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 183888-51-9 HCAPLUS

CN Glycine, N,N',N''-[[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 191537-47-0 HCAPLUS

CN Hexanoic acid,  $6,6',6''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino)]tris-, tris(phenylmethyl) ester, <math>(1\alpha,3\alpha,5\alpha)-(9CI)$  (CA INDEX NAME)

Relative stereochemistry.

RN 191537-48-1 HCAPLUS

CN Hexanoic acid, 6,6',6''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino)]tris-,  $(1\alpha,3\alpha,5\alpha)$ -(9CI) (CA INDEX NAME)

Relative stereochemistry.

$$HO_2C$$
 $(CH_2)_5$ 
 $HO_2C$ 
 $(CH_2)_5$ 
 $HO_2C$ 

IT 176839-96-6P 183888-57-5P 186031-88-9P 186031-89-0P 191537-50-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of collagen-like peptoid residue-containing triple helical structures)

RN 176839-96-6 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1\alpha,3\alpha,5\alpha)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4hydroxy- (9CI) (CA INDEX NAME)

# PAGE 1-B

PAGE 1-C

PAGE 2-B

RN 183888-57-5 HCAPLUS CN L-Prolinamide, 1,1',1''-[[(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-4-hydroxy-, (4R,4'R,4''R)- (9CI) (CA INDEX NAME)

#### PAGE 1-B

RN 186031-88-9 HCAPLUS

CN Glycinamide, 1,1',1''-[[(1α,3α,5α)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N2-(2-

methylpropyl) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 186031-89-0 HCAPLUS

# PAGE 1-B

PAGE 2-C

RN 191537-50-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1α,3α,5α)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycylN-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

PAGE 1-C

PAGE 2-A

L24 ANSWER 42 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1997:425133 HCAPLUS

#### Pryor 09 666463

DOCUMENT NUMBER: 127:77487

Collagen-Based Structures Containing the Peptoid TITLE: Residue N-Isobutylglycine (Nleu): Conformational

Analysis of Gly-Nleu-Pro Sequences by 1H-NMR and

Molecular Modeling

Melacini, Giuseppe; Feng, Yangbo; Goodman, Murray AUTHOR (S):

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343,

SOURCE:

Biochemistry (1997), 36(29), 8725-8732

CODEN: BICHAW; ISSN: 0006-2960

American Chemical Society PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

Mol. modeling and 1H-NMR were employed to study the structure and ΔR stability of collagen-like triple helixes composed of Gly-Nleu-Pro

repeats. The compds. studied include the acetyl analogs

Ac-(Gly-Nleu-Pro)n-NH2 (where n = 1, 3, 6, and 10) and the KTA conjugates KTA-[Gly-(Gly-Nleu-Pro)n-NH2]3 (where n=3 and 6 and KTA denotes the Kemp triacid). The presence of collagen-like assembled structures is supported by a consistent set of exptl. observations, which include the appearance of a distinct set of resonances, low hydrogen-exchange rates for Gly NH, cooperative melting transition, and observation of several interchain NOEs. Using 1H-NMR, the triple helicity was monitored as a function of

chain length, template, and temperature These studies show that

(Gly-Nleu-Pro)n

sequences have a somewhat higher triple-helical propensity than (Gly-Pro-Nleu)n sequences. In addition, our investigations have shown that unlike the triple helixes composed of Gly-Pro-Nleu repeats those composed of Gly-Nleu-Pro repeats can access conformations in which the Nleu side chains are arrayed between Pro residues belonging to different triple-helix cross sections. These structural features may serve as a basis for free energy computations and for the study of higher-order structures such as collagen-like fibrils containing peptoid moieties.

TΤ 191537-50-5

RL: PRP (Properties)

(conformational anal. of collagen-based Gly-Nleu-Pro sequences containing the peptoid residue N-isobutylqlycine (Nleu) by 1H-NMR and mol. modeling)

RN 191537-50-5 HCAPLUS

L-Prolinamide,  $1,1',1''-[[(1\alpha,3\alpha,5\alpha)-1,3,5-trimethy]-$ CN 1,3,5-cyclohexanetriyl]tricarbonyl]tris[qlycylqlycyl-N-(2methylpropyl)qlycyl-L-prolylqlycyl-N-(2-methylpropyl)qlycyl-L-prolylqlycyl-N-(2-methylpropyl)qlycyl- (9CI) (CA INDEX NAME)

# PAGE 1-B

PAGE 1-C

PAGE 2-A

L24 ANSWER 43 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:425132 HCAPLUS

DOCUMENT NUMBER: 127:77486

TITLE: Collagen-Based Structures Containing the Peptoid

Residue N-Isobutylglycine (Nleu): Synthesis and Biophysical Studies of Gly-Nleu-Pro Sequences by

Circular Dichroism and Optical Rotation

AUTHOR(S): Feng, Yangbo; Melacini, Giuseppe; Goodman, Murray

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of California at San Diego, La Jolla, CA, 92093-0343,

USA

SOURCE: Biochemistry (1997), 36(29), 8716-8724

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB Single-chain peptide-peptoid structures, Ac-(Gly-Nleu-Pro)n-NH2 (n = 3, 6, and 10) and (Gly-Nleu-Pro)n-NH2 (n = 1 and 9), and template-assembled collagen analogs, KTA-[Gly-(Gly-Nleu-Pro)n-NH2]3 (n = 3 and 6; KTA represents cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid, also known as the Kemp triacid; Nleu denotes N-isobutylglycine), were prepared by solid-phase peptide synthesis methods. Biophys. studies using CD and optical rotation measurements show that these collagen analogs form triple-helical conformations when the chain is longer than a critical length. Unlike collagen-based structures composed of Gly-Pro-Hyp and Gly-Pro-Nleu

sequences, results reveal that the presence of a pos. CD peak between 220 and 225 nm is indicative of triple-helical conformations for these collagen-based structures composed of Gly-Nleu-Pro sequences. Results also indicate that the Gly-Nleu-Pro sequence possesses a higher triple-helical propensity than the Gly-Pro-Nleu sequence as demonstrated by the higher melting temps., the faster triple-helix folding, and the lower min. concentration necessary to detect triple-helicity for the single-chain

structures. Therefore, we conclude that the Nleu residue in the second position of the trimeric repeat is more effective in inducing triple-helix formation than Pro in the same position.

IT 191537-50-5P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (synthesis and triple-helical propensities of collagen-based structures containing the peptoid residue N-isobutylglycine (Nleu) in Gly-Nleu-Prosequences)

RN 191537-50-5 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1α,3α,5α)-1,3,5-trimethyl 1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2 methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl N-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 1-C

PAGE 2-A

L24 ANSWER 44 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1997:175440 HCAPLUS

#### Pryor 09 666463

DOCUMENT NUMBER:

126:309200

TITLE:

Small molecular gelling agents to harden organic

liquids: trialkyl cis-1,3,5-cyclohexanetricarboxamides

AUTHOR (S):

Hanabusa, Kenji; Kawakami, Atsushi; Kimura, Mutsumi;

Shirai, Hirofusa

CORPORATE SOURCE:

Faculty of Textile Science & Technology, Shinshu

University, Ueda, 386, Japan

SOURCE:

Chemistry Letters (1997), (3), 191-192

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER:

Nippon Kagakkai

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Trialkyl cis-1,3,5-cyclohexanetricarboxamides were able to cause phys. AB gelation in organic liqs. to afford completely transparent organogel. main driving force for gelation was intermol. hydrogen bonding between amides and van der Waals interaction among hydrophobic alkyl chains.

189299-28-3 189299-29-4 189299-30-7 IT

189301-40-4

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(phys. gelation of trialkyl cis-1,3,5-cyclohexanetricarboxamides in organic liqs.)

189299-28-3 HCAPLUS RN

1,3,5-Cyclohexanetricarboxamide, N,N',N''-trihexyl-, CN  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_5$$
  $N$   $H$   $(CH_2)_5$   $M$   $H$ 

189299-29-4 HCAPLUS RN

1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, CN  $(1\alpha, 3\alpha, 5\alpha)$  - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{11}$$
  $N$   $H$   $(CH_2)_{11}$   $M$   $H$ 

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 
$$(CH_2)_{17}$$
  $(CH_2)_{17}$   $(CH_2)_{17}$ 

RN 189301-40-4 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,  $(1\alpha,3\alpha,5\alpha)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

-- CHMe2

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 45 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1997:143376 HCAPLUS

DOCUMENT NUMBER:

126:222195

TITLE:

Model molecules for the active center of alcohol

dehydrogenases-An FT-IR study

AUTHOR (S):

Brzezinski, Bogumil; Urjasz, Hanna; Zundel, Georg;

Bartl, Franz

CORPORATE SOURCE:

Faculty of Chemistry, Adam Mickiewicz University,

Poznan, 60 780, Pol.

SOURCE:

Biochemical and Biophysical Research Communications

#### Pryor 09 666463

(1997), 231(2), 473-476

CODEN: BBRCA9; ISSN: 0006-291X

PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We synthesized a triamide of Kemp's acid with two cysteine groups and one histidine group (compound 1), and a triamide of 1,3,5-pentane tricarboxylic acid with tyrosine, histidine, and arginine mols. (compound 2). From compound 1 we obtained the hydrated Zn2+ complex, compound 3. The FT-IR spectra of various complexes of compds. 1-3 with NAD+ show no IR continua and hence, no hydrogen-bonded chains with proton polarizability are present. In the case of the complex (compds. 2 and 3 and NAD+) an intense continuum demonstrates that a hydrogen-bonded chain is formed with large proton polarizability due to collective proton motion. This proton pathway is discussed. The O atom of the nicotinamide group of NAD+ is a strong hydrogen bond acceptor. This result is discussed with regard to the catalytic mechanism.

IT 188351-53-3P

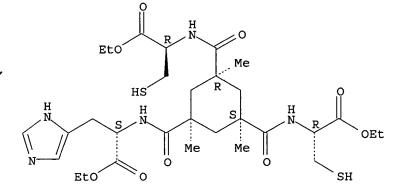
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(model mols. for the active center of alc. dehydrogenases-an FT-IR study)

RN 188351-53-3 HCAPLUS

CN L-Histidine, N-[[(1R,3R,5S)-3,5-bis[[[(1R)-2-ethoxy-1-(mercaptomethyl)-2-oxoethyl]amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 46 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:750209 HCAPLUS

DOCUMENT NUMBER: 126:118179

TITLE: Collagen-based structures containing the peptoid

residue N-isobutylglycine (NLeu): Synthesis and biophysical studies of Gly-Pro-NLeu sequences by circular dichroism, ultraviolet absorbance, and

optical rotation

AUTHOR(S): Feng, Yangbo; Melacini, Giuseppe; Taulane, Joseph P.;

Goodman, Murray

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of California San Diego, La Jolla, CA, 92093-0343, USA

SOURCE: Biopolymers (1996), 39(6), 859-872

CODEN: BIPMAA; ISSN: 0006-3525

PUBLISHER: Wiley

DOCUMENT TYPE: Journal LANGUAGE: English

A peptoid residue N-isobutylglycine (NLeu) was introduced as a proline AB surrogate in collagen-like triple helical structures. A series of single chain and template-assembled collagen-based peptide-peptoid structures composed of Gly-Pro-NLeu sequences were prepared by solid phase segment condensation methods. Both a synthetic route in solution and a solid phase method were employed to couple the KTA (cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid, also known as the Kemp triacid) based template, KTA-(Gly-OH)3 to peptide-peptoid chains. Biophys. studies using CD, UV, and optical rotation measurements demonstrated that these compds. form triple-helical structures when the chains are longer than critical lengths. Results from melting curve measurements indicated that the Gly-Pro-NLeu sequence is comparable to the Gly-Pro-Pro sequence in stabilizing a triple-helical conformation. The KTA-based template stabilized triple-helical structures as can be seen by the increased melting temps. as compared to equivalent single chain mols. In addition, the template reduced the min. chain length necessary to form a triple helix from six to only three trimer repeats.

IT 186031-88-9P 186031-89-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and biophys. properties of collagen-based structures containing isobutylglycine peptoid residues)

RN 186031-88-9 HCAPLUS

Absolute stereochemistry.

PAGE 1-A

$$H_2N$$
 $I-Bu$ 
 $I-Bu$ 

PAGE 1-B

RN 186031-89-0 HCAPLUS

CN Glycinamide, 1,1',1''-[[(1\alpha,3\alpha,5\alpha)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-(2-methylpropyl)glycylglycyl-L-prolyl-N-(2-methylpropyl)glycylglycyl-L-prolyl-N2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-A

PAGE 2-C

PAGE 2-B

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REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 47 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

USA

ACCESSION NUMBER:

1996:625561 HCAPLUS

DOCUMENT NUMBER:

126:15960

TITLE:

Collagen-Based Structures Containing the Peptoid Residue N-Isobutylglycine (Nleu): Conformational Analysis of Gly-Pro-Nleu Sequences by 1H NMR, CD, and

Molecular Modeling

AUTHOR(S):

Melacini, Giuseppe; Feng, Yangbo; Goodman, Murray Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343,

CORPORATE SOURCE:

SOURCE:

Journal of the American Chemical Society (1996),

118(44), 10725-10732

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER:

American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Mol. modeling, 1H NMR, and CD were employed to study the structure and AB stability of collagen-like triple helixes composed of Gly-Pro-Nleu repeats. The compds. studied include the acetyl analogs  $Ac^{-}(Gly-Pro-Nleu)n-NH2$  (where n = 1, 6, 9) and the KTA conjugates KTA-[Gly-(Gly-Pro-Nleu)n-NH2]3 (where n=1, 3, 6, 9 and KTA denotes the Kemp triacid). The presence of collagen-like assembled structures was supported by a consistent set of exptl. observations, including the appearance of a distinct set of resonances, low hydrogen exchange rates for Gly NH, KTA signal splitting, cooperative melting transition, and anal. of NOESY cross peaks. In this regard, the concept of ensemble interchain NOEs was introduced and used to establish the close packing of Gly, Pro, and Nleu residues in triple helixes composed of Gly-Pro-Nleu repeats. In addition, the ensemble interchain NOEs gave insight into the puckering of the Pro ring and the conformations accessible to the Nleu side chain. The effect of the KTA template on triple helicity was studied and shown to consist in a net gain in the free energy of triple-helix formation, as also seen for Gly-Pro-Hyp sequences. This free energy gain led to the induction of an assembled collagen-like structure in the KTA conjugate containing six Gly-Pro-Nleu repeats per chain and to an increase in thermal stability of the compound containing nine Gly-Pro-Nleu repeats per chain.

IT 184017-05-8 184017-06-9

RL: PRP (Properties)

(conformational anal. of collagen-like triple helixes composed of Gly-Pro-Nleu repeats)

RN 184017-05-8 HCAPLUS

CN L-Norleucinamide, 1,1',1''-[[( $1\alpha$ ,3 $\alpha$ ,5 $\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-methyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$\begin{array}{c|c} & & & \\ & & &$$

PAGE 1-C

PAGE 2-B

REFERENCE COUNT:

THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS 39 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2005 ACS on STN L24 ANSWER 48 OF 60

ACCESSION NUMBER:

1996:616678 HCAPLUS

DOCUMENT NUMBER:

126:75222

TITLE:

Acetyl-Terminated and Template-Assembled

Collagen-Based Polypeptides Composed of Gly-Pro-Hyp Sequences. 2. Conformational Analysis by 1H-NMR and

Molecular Modeling Studies

AUTHOR (S):

SOURCE:

CORPORATE SOURCE:

Melacini, Giuseppe; Feng, Yangbo; Goodman, Murray Department of Chemistry Biochemistry, University of

California, La Jolla, CA, 92093-0343, USA

Journal of the American Chemical Society (1996),

118(43), 10359-10364

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

#### Pryor 09 666463

DOCUMENT TYPE: Journal LANGUAGE: English

Using 1- and 2-dimensional 1H-NMR and mol. modeling, the conformational features of template-assembled collagen-like polypeptides of the type KTA-[Gly-(Gly-Pro-Hyp)n-NH2]3 (I; n = 1, 3, 5, 6; KTA=Kemp's triacid) and of the corresponding acetylated single-chain polypeptides Ac-(Gly-Pro-Hyp)n-NH2 (n = 1, 3, 5, 6, 9) were characterized in water. The presence of triple-helical conformations was established on the basis of consistent exptl. observations including the appearance of a set of distinct assembled resonances and the measurement of low hydrogen-exchange rates for the assembled Gly NH of the longer chain analogs. In addition, following the pioneering work of M.-H. Li, P. Fan, B. Brodsky, and J. Baum (1993), the consistency of the NOESY spectra with the interchain NOEs anticipated by the X-ray model for triple-helical (Gly-Pro-Hyp) sequences was proved. For I, the triple helicity is further supported by the KTA signal splitting detected for I (n = 3, 5, 6) and caused by the triple-helical screw symmetry which breaks the rotational symmetry of KTA. Thermal melting studies indicate that the KTA template leads to a significant gain in the free energy of triple-helix formation. This free energy gain results in a remarkable increase of the thermal stabilities of the KTA terminated compds. as compared to the acetyl analogs. The NMR results are fully consistent with the author's previous investigations based on CD, UV, and optical rotation spectroscopic methods.

IT 176839-96-6 183888-57-5

RL: PRP (Properties)

(conformational anal. of acetyl-terminated and template-assembled collagen-based polytripeptides by NMR and mol. modeling)

RN 176839-96-6 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1α,3α,5α)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4hydroxy- (9CI) (CA INDEX NAME)

# PAGE 1-B

PAGE 1-C

PAGE 2-B

PAGE 1-B

PAGE 2-A

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REFERENCE COUNT:

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

#### Pryor 09\_666463

L24 ANSWER 49 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:616677 HCAPLUS

DOCUMENT NUMBER: 126:75221

TITLE: Acetyl-Terminated and Template-Assembled

Collagen-Based Polypeptides Composed of Gly-Pro-Hyp Sequences. 1. Synthesis and Conformational Analysis by

Circular Dichroism, Ultraviolet Absorbance, and

Optical Rotation

AUTHOR(S): Feng, Yangbo; Melacini, Giuseppe; Taulane, Joseph P.;

Goodman, Murray

CORPORATE SOURCE: Department of Chemistry Biochemistry, University of

California at San Diego, La Jolla, CA, 92093-0343, USA

SOURCE: Journal of the American Chemical Society (1996),

118(43), 10351-10358

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Template-assembled collagen-based polypeptides KTA-[Gly-(Gly-Pro-Hyp)n-NH2]3 [I; n = 1, 3, 5, 6; KTA = cis,cis-1,3,5-trimethylcyclohexane-1,3,5tricarboxylic acid (Kemp's triacid)] and acetyl-terminated single-chain collagen-based analogs Ac-(Gly-Pro-Hyp)n-NH2 (II; n = 1, 3, 5, 6, 9) were synthesized by solid phase segment condensation methods. The triple-helical propensities of these collagen analogs were investigated using CD, UV absorbance, optical rotation, and NMR measurements. The acetyl analogs, II (n = 6, 9), assume a stable triple-helical conformation in H2O (0.2 mg/mL) at room temperature By contrast, II (n = 5) adopts a triple-helical conformation in H2O only below 18° at a concentration of 0.2 mg/mL. For the template-assembled collagen analogs, results show that I (n = 5, 6) peptides form triple-helical structures which have melting temps. above 70° in H2O. These melting temps. are much higher than those of the corresponding acetyl analogs, demonstrating the significant triple-helix-stabilizing effects of the KTA template. In addition, the KTA template facilitates triple-helical structures by dramatically accelerating triple-helix formation.

IT 176839-96-6P 183888-57-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and conformational anal. of acetyl-terminated and template-assembled collagen-based polytripeptides)

RN 176839-96-6 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1α,3α,5α)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4hydroxy- (9CI) (CA INDEX NAME)

# PAGE 1-B

PAGE 1-C

PAGE 2-B

PAGE 1-B

PAGE 2-A

N
S
N
OH

(preparation and conformational anal. of acetyl-terminated and template-assembled collagen-based polytripeptides)

RN 183888-50-8 HCAPLUS

CN Glycine, N,N',N''-[[( $1\alpha$ ,  $3\alpha$ ,  $5\alpha$ )-1,3,5-trimethyl-1,3,5-

cyclohexanetriyl]tricarbonyl]tris-, tris(phenylmethyl) ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 183888-51-9 HCAPLUS

CN Glycine, N,N',N''-[[( $1\alpha$ , $3\alpha$ , $5\alpha$ )-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$HO_2C$$
 $Me$ 
 $Me$ 
 $Me$ 
 $HO_2C$ 
 $Me$ 
 $Me$ 
 $HO_2C$ 
 $Me$ 
 $Me$ 
 $HO_2C$ 
 $M$ 

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 50 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:567102 HCAPLUS

DOCUMENT NUMBER: 125:197514

TITLE: Crystalline resin compositions

INVENTOR(S): Ikeda, Naoki; Yoshimura, Masafumi; Mizoguchi, Kazuaki;

Kitagawa, Hiroshi

PATENT ASSIGNEE(S): Shin Nippon Rika Kk, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

#### Pryor 09\_666463

JP 1995-170313 JP 08157640 A2 19960618 19950612

PRIORITY APPLN. INFO.: JP 1994-240112 A1 19941004

Crystalline resins contain 0.001-10 phr ≥1 amide selected from amides of polycarboxylic acids, polyamines, and poly(amino acids) to improve crystallization

rates. Thus, poly(phenylene sulfide) pellets containing 0.2 phr terephthalic acid dicyclohexylamide had crystallization temperature 230°, compared with 191° for the resin alone.

ŦΤ 160535-62-6

RL: MOA (Modifier or additive use); USES (Uses)

(crystalline resin compns. containing amides as nucleating agents)

RN160535-62-6 HCAPLUS

1,3,5-Cyclohexanetricarboxamide, N,N',N''-triphenyl- (9CI) (CA INDEX CN NAME)

L24 ANSWER 51 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:285056 HCAPLUS

DOCUMENT NUMBER: 124:336180

A Template-Induced Incipient Collagen-Like TITLE:

Triple-Helical Structure

AUTHOR (S): Goodman, Murray; Feng, Yangbo; Melacini, Giuseppe;

Taulane, Joseph P.

CORPORATE SOURCE: Department of Chemistry Biochemistry, University of

California, San Diego, La Jolla, CA, 92093-0343, USA

SOURCE: Journal of the American Chemical Society (1996),

118(21), 5156-5157

CODEN: JACSAT; ISSN: 0002-7863

American Chemical Society PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

A template-assembled polypeptide system that mimics the collagen-like triple helix is presented. A conformationally highly constrained organic structure, cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid (also known as the Kemp triacid, KTA) was used as a template to nucleate the triple helical folding of three polypeptide chains, each of which contains only three glycyl-prolyl-hydroxyprolyl (Gly-Pro-Hyp) repeats. These three chains were linked to the KTA through glycine residues which act as spacers. The resulting system KTA-[Gly-(Gly-Pro-Hyp)3-NH2]3 assumes a triple helical conformation in H2O at room temperature as verified by 1H-NMR and optical rotation. Our results indicate that the short helical structure adopted by KTA-[Gly-(Gly-Pro-Hyp)3-NH2]3 exhibits some cooperativity and is significantly affected by triple helix and effects. We therefore define this assembled conformation as an incipient triple To the best of our knowledge, this system represents the shortest chain collagen-like triple helical mol. which has been reported in the

literature.

IT 176839-96-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (a template-induced incipient collagen-like triple-helical structure, KTA-[Gly-(Gly-Pro-Hyp)3-NH2]3)

RN 176839-96-6 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1\alpha,3\alpha,5\alpha)-1,3,5-trimethyl1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4hydroxy- (9CI) (CA INDEX NAME)

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L24 ANSWER 52 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1995:825831 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 124:30376

TITLE: Kemp's triacid scaffolding for synthesis of

combinatorial nonpeptide uncoded libraries

AUTHOR (S): Kocis, Petr; Issakova, Olga; Sepetov, Nikolai F.;

Lebl, Michal

CORPORATE SOURCE: Chem. Dep., Selectide Corp., Tucson, AZ, 85737, USA

SOURCE: Tetrahedron Letters (1995), 36(37), 6623-6

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier DOCUMENT TYPE: Journal

Ι

LANGUAGE: English OTHER SOURCE(S): CASREACT 124:30376

GΙ

II

#### Pryor 09\_666463

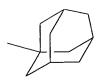
Synthesis of differentially protected mol. scaffold I (Boc = Me3CO2C; Fmoc AB = 9-fluorenylmethoxycarbonyl) for nonpeptide combinatorial libraries is described. Solid phase synthesis of model compds. II [R = PhCH2CH2CO, R1 = Ac, R3 = Lys(Admoc)-OH; R = Ac-Phe, R1 = Ac, R2 = Arg- $\beta$ -Ala-Gly- $\beta$ -Ala-Gly-OH; R = 6-amino-3-pyridinecarbonyl, R1 = 4-[HN:C(NH2)NH]C6H4CO,  $R2 = Arg-\beta-Ala-Gly-\beta-Ala-Gly-OH$ ; R =HO2CCH2CH2CO, R1 = 2-pyrazinecarbonyl, R2 =  $Asp-\beta-Ala-Gly-B-Ala-Gly-B-Ala-$ Gly-OH; Admoc = 1-adamantylmethoxycarbonyl] and a nonpeptide combinatorial library as well as the structure elucidation in the absence of coding is disclosed. 171563-25-0P 171563-26-1P 171563-27-2P IT 171563-28-3P 171563-30-7DP, diamide reaction products with carboxylic acid mixts. RL: SPN (Synthetic preparation); PREP (Preparation) (use of Kemp's triacid as a scaffold for the preparation of nonpeptide uncoded combinatorial libraries)

RN 171563-25-0 HCAPLUS

L-Lysine, N2-[[3-[[[2-(acetylamino)ethyl]amino]carbonyl]-1,3,5-trimethyl-5[[[2-[(1-oxo-3-phenylpropyl)amino]ethyl]amino]carbonyl]cyclohexyl]carbonyl
]-N6-[(tricyclo[3.3.1.13,7]dec-1-ylmethoxy)carbonyl]-,
(1α,3α,5α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B



RN 171563-26-1 HCAPLUS CN Glycine, N-[N-[N-[N-[N2-[[3-[[[2-(acetylamino)ethyl]amino]carbonyl]-5-[[[2[{2-(acetylamino)-1-oxo-3-phenylpropyl]amino]ethyl]amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-L-arginyl]- $\beta$ -alanyl]glycyl]- $\beta$ -alanyl]-, [1S-[1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 171563-27-2 HCAPLUS

CN Glycine, N-[N-[N-[N-[N2-[[3-[[[2-[[4-[(aminoiminomethyl)amino]benzoyl]amin o]ethyl]amino]carbonyl]-5-[[[2-[[(6-amino-3-pyridinyl)carbonyl]amino]ethyl]amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-L-arginyl]- $\beta$ -alanyl]glycyl]- $\beta$ -alanyl]-, [1S-(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )]- (9CI) (CA INDEX NAME)

$$H_2N$$
 $H_2N$ 
 $H_2N$ 
 $H_3N$ 
 $H_4N$ 
 $H_4N$ 
 $H_5N$ 
 $H_5N$ 
 $H_5N$ 
 $H_6N$ 
 $H_7N$ 
 $H_7N$ 

#### PAGE 1-B

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RN 171563-28-3 HCAPLUS Glycine, N-[N-[N-[N-[N-[[3-[[[2-[(3-carboxy-1-oxopropyl)amino]ethyl]amino]carbonyl]-1,3,5-trimethyl-5-[[[2-[(pyrazinylcarbonyl)amino]ethyl]amino]carbonyl]cyclohexyl]carbonyl]-L-\alpha-aspartyl]-\beta-alanyl]glycyl]-\beta-alanyl]-, [1S-(1\alpha,3\alpha,5\alpha)]- (9CI) (CA INDEX NAME)
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PAGE 1-B

RN 171563-30-7 HCAPLUS

CN Glycine, N-[N-[N-[N-[[3,5-bis[[(2-aminoethyl)amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]- $\beta$ -alanyl]glycyl]- $\beta$ -alanyl]-, (1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

M CO2H

L24 ANSWER 53 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:644496 HCAPLUS

DOCUMENT NUMBER:

123:284942

TITLE:

Hydrogen-bonding control of molecular aggregation:

self-complementary subunits lead to rod-shaped

structures in the solid state

AUTHOR (S):

Fan, Erkang; Yang, Ji; Geib, Steven J.; Stoner,

Timothy C.; Hopkins, Michael D.; Hamilton, Andrew D. Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260,

IICA

CORPORATE SOURCE:

Journal of the Chemical Society, Chemical

Communications (1995), (12), 1251-2

CODEN: JCCCAT; ISSN: 0022-4936

PUBLISHER:

SOURCE:

Royal Society of Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB Simple cyclohexane-1,3,5-triamide derivs. (e.g. I) are shown to form linear, rod-shaped structures in the solid state; a triple hydrogen-bonding interaction directs formation of the aggregate and leads to non-centrosym. packing arrangement with modest nonlinear optical properties.

Ι

IT 169557-72-6

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

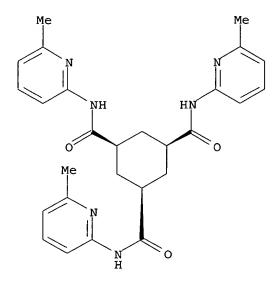
### Pryor 09 666463

(hydrogen-bonding control of mol. aggregation in cyclohexane-1,3,5triamide derivs.)

RN 169557-72-6 HCAPLUS

1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(6-methyl-2-pyridinyl)-, CN $(1\alpha, 3\alpha, 5\alpha)$  - (9CI)(CA INDEX NAME)

Relative stereochemistry.



L24 ANSWER 54 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:550045 HCAPLUS

DOCUMENT NUMBER:

123:256099

TITLE:

A cyclohexane spacer for phosphate receptors

AUTHOR (S):

Raposo, Cesar; Perez, Nieves; Almaraz, Marta; Mussons,

M. Luisa; Caballero, M. Cruz; Moran, Joaquin R.

CORPORATE SOURCE:

Dep. Quim. Org., Univ. Salamanca, Salamanca, E-37008,

Spain

SOURCE:

Tetrahedron Letters (1995), 36(18), 3255-8

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

DOCUMENT TYPE:

Elsevier Journal

LANGUAGE:

English

GΙ

AB A cyclohexanetricarboxylic acid is shown to be a good spacer for phosphate guests. The combination of 8-aminochromenone-2-carboxamide groups with the cyclohexane spacer leads to a versatile receptor (I), which sets six hydrogen bonds with either phosphonic acids or phosphates. Large association consts. are obtained for this receptor in DMSO and methanol when tetraalkylammonium phosphates are used as guests.

Ι

IT 168705-28-0P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (hydrogen bonded with phenylphosphonic acid; cyclohexane spacer for phosphate receptors)

RN 168705-28-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[(butylamino)carbonyl]-6-(1,1-dimethylethyl)-4-oxo-4H-1-benzopyran-8-yl]-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 2-A

IT 168705-27-9P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (hydrogen bonded with propylphosphonic acid; cyclohexane spacer for phosphate receptors)

RN 168705-27-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(1,1,3,3-tetramethylbutyl)-,  $(1\alpha,3\alpha,5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L24 ANSWER 55 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:543429 HCAPLUS

DOCUMENT NUMBER: 122:267113

TITLE: Polyamide and amide compound compositions with good

degree of crystallinity

INVENTOR(S): Kitagawa, Hiroshi; Yana, Yoshitaka; Mizoguchi,

Kazuaki; Kawahara, Yasuyuki; Sadamitsu, Kyoshi;

Yoshimura, Masafumi; Ikeda, Naoki

PATENT ASSIGNEE(S): Shin Nippon Rika KK, Japan; New Japan Chemical Co.,

Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06271762	A2	19940927	JP 1994-15830	19940113
JP 3477787	B2	20031210		
JP 2004035895	A2	20040205	JP 2003-290992	20030811
PRIORITY APPLN. INFO.:			JP 1993-26179	A 19930120
			JP 1994-15830	A3 19940113

OTHER SOURCE(S): MARPAT 122:267113

AB The compns. comprise a polyamide and a compound selected from polycarboxylic acid amide, polyamine polyamide and/or polyamino amide. A composition from nylon 6 containing 0.2 phr N,N'-dicyclohexylterephthalamide showed degree of crystallinity 182°.

IT 162957-51-9

RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)

(polyamide and amide compound compns. with good degree of crystallinity)

RN 162957-51-9 HCAPLUS

CN Cyclohexanecarboxamide, 3,5-bis[(cyclohexylcarbonyl)amino]-N-phenyl- (9CI) (CA INDEX NAME)

L24 ANSWER 56 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:118642 HCAPLUS

DOCUMENT NUMBER: 122:107612

TITLE: Crystalline propylene polymer compositions with

excellent rigidity

INVENTOR(S): Mizoguchi, Kazuaki; Yoshimura, Masafumi; Ikeda, Naoki;

Sadamitsu, Kyoshi; Kawahara, Yasuyuki; Yana,

Yoshitaka; Kitagawa, Hiroshi

PATENT ASSIGNEE(S): Shin Nippon Rika Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

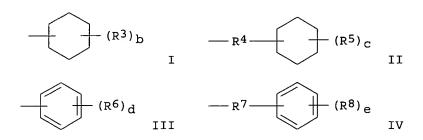
CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192496	A2	19940712	JP 1993-269840	19930930
JP 3401868	B2	20030428		
PRIORITY APPLN. INFO.:			JP 1992-308233	A1 19921022



AB The compns. contain ≥1 R1(CONHR2)a [R1 = aliphatic, alicyclic, or aromatic polycarboxylic acid residue; R2 = (cyclo)alkyl, (cyclo)alkenyl, Ph, naphthyl, I, II, III, IV; R3, R5, R6, R8 = independently (cyclo)alkyl, alkenyl, alkoxy, Ph, halo; R4, R7 = linear or branched alkylene; a = 3-6; b, d = 1-5; c, e = 0-5]. Thus, 100 parts ethylene-propylene block copolymer (melt flow rate 2 g/10-min) and 0.2 part biphenyltetracarboxylic acid tetracyclohexylamide were melt kneaded and pelletized to give a composition showing crystallization temperature 125° for its press sheet and flexural

modulus 11,300 kg/cm2 for its injection molded test piece.

IT 160535-62-6 160535-63-7

RL: MOA (Modifier or additive use); USES (Uses)

(amide additives for rigid crystalline propylene polymers)

RN 160535-62-6 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-triphenyl- (9CI) (CA INDEX

NAME)

RN 160535-63-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tricyclohexyl- (9CI) (CA INDEX NAME)

L24 ANSWER 57 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:32622 HCAPLUS

DOCUMENT NUMBER: 122:31918

TITLE: Structure-activity relationships of double-strand RGD

peptides as GPIIb/IIIa receptor antagonists

AUTHOR(S): Ojima, Iwao; Dong, Qing; Eguchi, Masakatsu; Oh,

Young-im; Amann, Clare M.; Coller, Barry S.

CORPORATE SOURCE: School. Medicine, State University New York, Stony

Brook, NY, 11794, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1994),

4(14), 1749-54

CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Journal LANGUAGE: English

AB A series of new double-strand RGD peptides M(CO-Arg-Gly-Asp-Phe-OH)2 [M = (CH2)n, p-C6H4, n = 2-4] and (R-Arg-Gly-Asp-Phe-NH)2XZ [R = H, Me(CH2)4CO,

Bz, 4-[HN:C(NH2)NH]C6H4CO-Ser; X = Lys, Orn, cis,cis-3,5diaminocyclohexanecarbonyl, 3,5-(Gly-NH)2C6H3CO; Z = NH2,

Gly-Arg-Gly-Asp-Phe-NH2, Arg-Gly-Asp-Phe-OH] were prepared and their

inhibitory activities evaluated for platelet aggregation. Substantial improvement in activity is observed with these novel RGD peptides in comparison with single-strand RGD peptides. The structure-activity relationships of these double-strand RGD peptides are discussed.

IT 159652-31-0P 159652-32-1P 159652-33-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and blood platelet aggregation inhibitory activity of) 159652-31-0 HCAPLUS

Absolute stereochemistry.

PAGE 1-B

RN 159652-32-1 HCAPLUS

CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-(N-L-arginylglycyl)-L- $\alpha$ -aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbonyl]-L-arginyl]glycyl]-L- $\alpha$ -aspartyl]-, [3R-(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )]- (9CI) (CA INDEX NAME)

### PAGE 1-B

RN 159652-33-2 HCAPLUS

CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-[N-(N2-benzoyl-L-arginyl)glycyl]-L- $\alpha$ -aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbon yl]-L-arginyl]glycyl]-L- $\alpha$ -aspartyl]-, [3R-(1 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ )]- (9CI) (CA INDEX NAME)

PAGE 1-B

L24 ANSWER 58 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:208601 HCAPLUS

DOCUMENT NUMBER: 120:208601

TITLE: Platelet aggregation inhibitors that prevent the

#### Pryor 09\_666463

interaction of platelets and fibrinogen

INVENTOR(S): Ojima, Iwao; Eguchi, Masakatsu; Oh, Young Im; Coller,

Barry S.

PATENT ASSIGNEE(S): Research Foundation of State University of New York,

USA

SOURCE: PCT Int. Appl., 10 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATEN	T NO.			KINI	כ	DATE		i	APPL	ICAT:	ION 1	NO.		D	ATE	
		<del>-</del> -			-									-		
WO 94	00144			A1		1994	0106	1	WO 1	993-1	JS61	50		1:	9930	629
W	: AT,	ΑU,				CA,	CH,	CZ,	DE,	DK,	ES,	FI,	GB,	HU,	JP,	KΡ,
	KR,	LK,	LU,	MG,	MN,	MW,	NL,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SK,
		VN														
R	W: AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,
	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	MR,	NE,	SN,	TD,	TG		
US 53	38725			Α		1994	0816	1	US 1	992-	9065	25		1:	9920	630
AU 93	46544			A1		1994	0124	1	AU 1	993-4	4654	4		1	9930	629
PRIORITY A	PPLN.	INFO	. :					1	US 1	992-	9065:	25	i	A 1:	9920	630
								1	WO 1	993-1	US61	50	i	A 1:	9930	629

AB Synthetic peptides containing the RGD adhesion tripeptide are prepared for use as platelet aggregation inhibitors. The RGD peptide is flanked by by other short peptides, optionally including a alkyl, cycloalkyl, aromatic, or heteroarom. terminal extensions and has reactive carboxyl and amino termini for the formation of oligomers that give high local concns. of the RGD peptide. The peptide (RGPFPG) 2Dab-G-OH was synthesized by Fmoc chemical to give the TFA salt, this was converted to the acetate by ion-exchange and the acetate inhibited the ability of platelet-rich plasma to aggregate with an adjusted IC50 of 6.7+10-7 M. Thirty-one peptides in accordance with the invention were synthesized and their adjusted IC50's were in the range 7.6+10-8 - 4.4+10-6 M.

IT 154207-63-3P 154207-72-4P 154207-88-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, platelet aggregation inhibition by)

RN 154207-63-3 HCAPLUS

CN L-Phenylalaninamide, L-arginylglycyl-L-α-aspartyl-N-[3-(aminocarbonyl)-5-[[N-[N-(N-L-arginylglycyl)-L-α-aspartyl]-Lphenylalanyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 154207-72-4 HCAPLUS

CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-(N-L-arginylglycyl)-L- $\alpha$ -aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbonyl]-L-arginyl]glycyl]-L- $\alpha$ -aspartyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 154207-88-2 HCAPLUS

CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-[N-(N2-benzoyl-L-arginyl)glycyl]-L-α-aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbon yl]-L-arginyl]glycyl]-L-α-aspartyl]- (9CI) (CA INDEX NAME)

## PAGE 1-B

PAGE 2-B

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### Pryor 09\_666463

L24 ANSWER 59 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:192086 HCAPLUS

DOCUMENT NUMBER: 120:192086

TITLE: Preparation of bile acid derivatives as hypolipemics INVENTOR(S):

Enhsen, Alfons; Glombik, Heiner; Kramer, Werner; Wess,

Guenther

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Eur. Pat. Appl., 32 pp. CODEN: EPXXDW

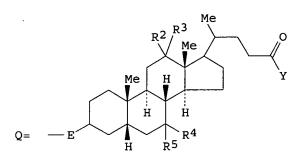
Patent DOCUMENT TYPE: German LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

GI

PATENT NO.		DATE	APPLICATION NO.	DATE	
	A2		EP 1993-108559	19930527	
EP 573848			BB, GR, IE, IT, LI, LU	J. MC. NI. PT.	SE
			AT 1993-108559		
ES 2111092	Т3	19980301	ES 1993-108559	19930527	
US 5428182	A	19950627	US 1993-74753	19930610	
IL 105980	A1	19971120	IL 1993-105980	19930610	
CZ 285104	B6	19990512	CZ 1993-1134	19930610	
SK 280819	B6	20000814	SK 1993-585	19930610	
FI 106801	B1	20010412	FI 1993-2659	19930610	
CA 2098256	AA	19931213	CA 1993-2098256	19930611	
CA 2098256	C	20040824			
NO 9302159	Α	19931213	NO 1993-2159	19930611	
AU 9340180	A1	19931216	AU 1993-40180	19930611	
AU 663592	B2	19951012			
ZA 9304150	Α	19940113	ZA 1993-4150	19930611	
HU 64772	A2	19940228	HU 1993-1716	19930611	
HU 216636	В	19990728			
JP 06087884	A2	19940329	JP 1993-140375	19930611	
JP 3403218	B2	20030506			
PRIORITY APPLN. INFO.:			DE 1992-4219274	A 19920612	
OTHER SOURCE(S):	MARPAT	120:192086	5		
CT					



Z(XG)n (G = bile acid residue, e.g., Q; E = bond, O, NH; R2-R5 = H, OH, AB alkoxy, NH2, alkanoyloxy, etc.; X = bond, bridging group; Y = OH, alkoxy, NH2, etc.; Z = n-valent group; n = 3 or 4) were prepared Thus, MeC(CH2OCH2CH2COR7)3 (I; R7 = OH) was condensed with RCH2CH2NH2 (R = Q; E

#### Pryor 09 666463

 $= \beta - O$ ,  $R2 = R4 = \alpha - OH$ , R3 = R5 = H, Y = OR6) (Q1; R6 = Me) to qive, after saponification, I (R7 = NHCH2CH2Q1; R6 = H) which had IC50 0.24 that of taurochenodesoxycholate for inhibition of taurocholate uptake by rabbit ileal vesicles in vitro. IT 153582-90-2P 153582-91-3P 153582-97-9P 153582-98-0P 153582-99-1P 153583-03-0P 153583-04-1P 153583-05-2P 153583-06-3P 153583-07-4P 153583-08-5P 153583-09-6P 153583-11-0P 153583-12-1P 153583-13-2P 153665-88-4P 153665-89-5P 153665-90-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as hypolipemic) RN 153582-90-2 HCAPLUS CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5cyclohexanetriyl) tris (carbonylimino-6,1-hexanediyloxy)] tris [7,12-dihydroxy-, trimethyl ester, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 2-A

153582-91-3 HCAPLUS RN

Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-CN cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-B

Me 
$$R$$
 H  $R$  H  $R$ 

PAGE 2-A

H OH

RN 153582-97-9 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[1,3,5-cyclohexanetriyltris(carbonylimino-2,1-ethanediyl)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

H !

PAGE 2-B

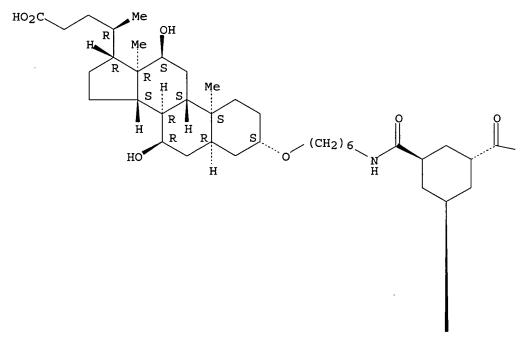
RN 153582-98-0 HCAPLUS

CN Cholan-24-oic acid, 3,3',3''-[1,3,5-cyclohexanetriyltris(carbonylimino-2,1-ethanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-B

RN 153582-99-1 HCAPLUS

CN Cholan-24-oic acid, 3,3',3''-[1,3,5-cyclohexanetriyltris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)



PAGE 1-B

H

PAGE 2-B

RN 153583-03-0 HCAPLUS

PAGE 1-B

PAGE 2-A

H OH

Me

PAGE 2-B

RN 153583-05-2 HCAPLUS

CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-5,1-pentanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 2-A

H OH

Absolute stereochemistry.

PAGE 2-A

Me

RN 153583-07-4 HCAPLUS

CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-2,1-ethanediyloxy-2,1-ethanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-C

\_\_CO2H

PAGE 2-A
H OH
Me

Absolute stereochemistry.

PAGE 1-A

## PAGE 1-B

# PAGE 1-C

PAGE 2-C

RN 153583-09-6 HCAPLUS

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 153583-11-0 HCAPLUS

CN Cholan-24-oic acid, 3,3'-[[5-[[[2-[(7,12-dihydroxy-24-methoxy-24-oxocholan-3-yl)oxy]ethyl]amino]carbonyl]-1,3,5-trimethyl-1,3cyclohexanediyl]bis(carbonylimino-6,1-hexanediyloxy)]bis[7,12-dihydroxy-, dimethyl ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 2-B

OMe

OMe

RN 153583-12-1 HCAPLUS
CN Cholan-24-oic acid, 3,3'-[[5-[[[2-[(23-carboxy-7,12-dihydroxy-24-norcholan-3-yl)oxy]ethyl]amino]carbonyl]-1,3,5-trimethyl-1,3-cyclohexanediyl]bis(carbonylimino-6,1-hexanediyloxy)]bis[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## PAGE 1-A

# PAGE 1-B

PAGE 2-A

RN 153583-13-2 HCAPLUS

CN Cholan-24-oic acid, 3,3'-[[5-[[[6-[[24-[[6-[(23-carboxy-7,12-dihydroxy-24-norcholan-3-yl)oxy]hexyl]amino]-7,12-dihydroxy-24-oxocholan-3-yl]oxy]hexyl]amino]carbonyl]-1,3,5-trimethyl-1,3-cyclohexanediyl]bis(carbonylimino-6,1-hexanediyloxy)]bis[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

## PAGE 1-B

PAGE 1-C

Me HO Me R H 
$$(CH_2)_6$$

N  $(CH_2)_6$ 

N  $(CH_2)_6$ 

N  $(CH_2)_6$ 

N  $(CH_2)_6$ 

N  $(CH_2)_6$ 

N  $(CH_2)_6$ 

OH

RN 153665-88-4 HCAPLUS

CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, trisodium salt, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 2-A

H OH

●3 Na

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

H OH

PAGE 2-A

RN 153665-90-8 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 2-A

H OH

L24 ANSWER 60 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:55386 HCAPLUS

DOCUMENT NUMBER: 72:55386

TITLE: Compounds with urotropine structure. XLV.

Cyclizations starting from 1,3,5-triaminocyclohexane

AUTHOR(S): Stetter, Hermann; Theisen, Dieter; Steffens, Gerd J.

CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Aachen, Aachen, Fed.

Rep. Ger.

SOURCE: Chemische Berichte (1970), 103(1), 200-4

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 72:55386

GI For diagram(s), see printed CA Issue.

AB 1,3,5-(O2N)3C6H3 was hydrogenated on Pd/C in AcOEt and R2O to 1,3,5-(RNH)3C6H3 which on further hydrogenation gave .apprx.20% trans and 80% cis isomers of cyclohexanes (I) [where R = Ac or EtCO (Ia)]. trans-Ia

was converted with HC(OEt)3 at 265° to the 2,4,10-triazaadamantane (II) (R = EtCO). This on saponification gave pure cis-I (R = H). Both cis-

and

trans-I (R = PhSO2), obtained from I (R = H) with PhSO2Cl, and CH(OEt)3 were similarly converted to II (R = PhSO2). However, PhSO2NHMe and CH(OEt)3 gave (PhSO2NMe)2CH(OEt).

IT 26159-21-7P 26159-22-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 26159-21-7 HCAPLUS

CN Propionamide, N,N',N''-1,3,5-cyclohexanetriyltris-, cis, cis- (8CI) (CA INDEX NAME)

RN 26159-22-8 HCAPLUS
CN Propionamide, N,N',N''-1,3,5-cyclohexanetriyltris-, stereoisomer (8CI)
(CA INDEX NAME)

=> => d stat que 126 L12 STR

O<u></u>C ∼ NH 17 @18 19



28 O |||| S~~ C @25 26 0<u></u> C ∼ S 13 @14 15

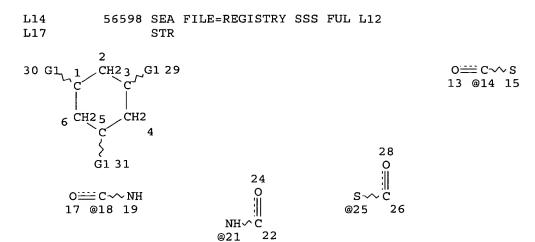
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GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE



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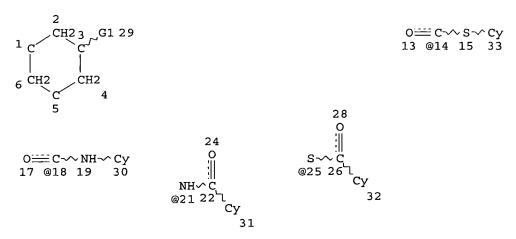
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L20 STF



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GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L21 STR

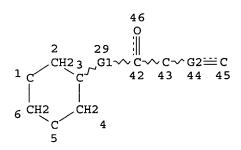
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GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE L22 STR



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GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L23 145 SEA FILE=REGISTRY SUB=L18 SSS FUL L21 OR L22 OR L20

L24 60 SEA FILE=HCAPLUS ABB=ON PLU=ON L23

L25 39 SEA FILE=HCAPLUS ABB=ON PLU=ON ("LIVOREIL A"/AU OR "LIVOREIL

AUDE"/AU)

L26 37 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 NOT L24

=> d ibib abs hitstr 126 1-37

L26 ANSWER 1 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2005:1145996 HCAPLUS

TITLE:

Permanent hair shaping composition containing a

reducing agent and a photo-oxidant

INVENTOR(S): Livoreil, Aude; Vic, Gabin; Samain, Henri

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

P	ΓA	ENT	NO.			KIN	D	DATE		1	APPL	ICAT	ION I	NO.	D	ATE	
- E	EP 1588691					 A1	-	 2005	1026	•	 EP 2	 005-:	 3003	01	 2	 0050	 420
		R:			LT,	LV,		ES, RO,									

PRIORITY APPLN. INFO.:

FR 2004-50764

A 20040422

חתיים

AB Unavailable

L26 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:1067500 HCAPLUS

DOCUMENT NUMBER:

143:352825

TITLE:

Hair-perming composition comprising at least one

ADDITENTED NO

metal-modified material

INVENTOR(S):

Livoreil, Aude; Vic, Gabin; Samain, Henri

PATENT ASSIGNEE(S):

L'Oreal, Fr.

SOURCE:

Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

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DOCUMENT TYPE:

Patent

LANGUAGE:

French

KIND

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	T.EW.L	NO.			KIN		DATE		F	APP.	LICAT	TON I	NO.		L	ATE	
						-			-						-		
EP	1582	199			A1		2005	1005	I	ΞP	2005-	3002:	29		2	0050	330
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		ΙE,	SI,	LT,	LV,	FΙ,	RO,	MK,	CY,	AL	, TR,	BG,	CZ,	EE,	HU,	PL,	SK,
		ВA,	HR,	IS,	ΥU												
FR	2868	303			<b>A</b> 1		2005	1007	I	FR :	2004-	5064:	2		2	0040	331
FR	2868	302			A1		2005	1007	I	FR :	2004-	9259			2	0040	901
CA	2502	998			AA		2005	0930	(	CA	2005-	2502	998		2	0050	330
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PRIORIT	Y APP	LN.	INFO	. :					I	'R	2004-	50642	2	1	A 2	0040	331
									I	R:	2004-	9259		1	A 2	0040	901
									τ	JS :	2004-	5721	05P	]	P 2	0040	519

AB An aqueous reducing composition for permanent hair wave preparation contains a reducing

agent, a material modified by incorporation of an oxidant chosen from transition metals in the form of salts, oxides or complexes with a ligand. A reducing composition for permanent hair wave prepns. contained thioglycolic acid 9, Zeostop X (comprising Cu, Zn, and Ag) 5, 20% ammonia (pH 9), and water qs to 100 g.

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2005:1025551 HCAPLUS

DOCUMENT NUMBER:

143:332027

TITLE: Cosmetic compositions containing modified polyamines

and uses of the compositions

INVENTOR(S): Livoreil, Aude; Vic, Gabin

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 40 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	PATENT NO.					<b>)</b>	DATE		i			ION 1			D	ATE		
FR :	 2867	 679			A1	-	2005	0923	]			 5053:			20	0040	 317	
WO :	2005	0922	74		A1		2005	1006	1	WO 2	005-	FR50	169		. 20	0050	316	
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
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		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	ΚZ,	LC,	
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		MR,	ΝE,	SN,	TD,	TG												
RITY	ITY APPLN. INFO.:									FR 2	004-	5053	2	1	A 20	0040	317	

PRIORITY APPLN. INFO.:

FR 2004-50532

A 20040317

AB The compns. useful for imparting softness to keratin material or hair, are prepared in aqueous medium and contain cosmetic-acceptable polymers bearing ≥2 linear NH or/and branching N groups on main chain while lacking of vinylamine or vinylamide group, where the polymers are modified with ≥1 hydrophilic or/and hydrophobic hydrocarbyl segments and do not contain group of S, Si or amidino, the hydrophilic segments are different from sugar, and the modification with hydrophobic segments is not done via a bifunctional spacing group. Thus, mixing a 10% aqueous solution of Lupasol P (aziridine polymer) at pH 8.5 with an 10% aqueous solution of glucose in the presence of a NaBH3CN gave a modified polyamine.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:467779 HCAPLUS

DOCUMENT NUMBER: 142:487139

TITLE: Cosmetic composition for forming a polymeric matrix

with hollow embossments or outgrowths

INVENTOR(S): Vic, Gabin; Livoreil, Aude; Samain, Henri;

Heinzelmann, Harry; Pugin, Rapha L.; Jeney, Sylvia

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ENT	NO.			KINI	)	DATE			APPL:	ICAT:	ION I	. 01		D	ATE		
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ΕP	1535	608			A1		2005	0601	:	EP 2	004-	2925	32		2	0041	026	
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		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR

FR 2862869 A1 20050603 FR 2003-50935 20031128
US 2005129646 A1 20050616 US 2004-990880 20041118
JP 2005162753 A2 20050623 JP 2004-342820 20041126
PRIORITY APPLN. INFO.: FR 2003-50935 A 20031128
US 2004-562554P P 20040416
AB A cosmetic composition comprises n number of polymers (P1, P2...Pn) with

10≥n≥2 solubilized in a solvent (S). The polymers (P1, P2...Pn) and the solvent (S) which is liquid at room temp and pressure can form a distinctive domains constituted by each polymer alone after deposition on the human hair and evaporation of the solvent. A hair

contained polystyrene 2, polymethyl methacrylate 1, and toluene q.s. 100

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:586 HCAPLUS

DOCUMENT NUMBER: 142:79556

TITLE: Cosmetic composition with a nitrosonium salt for the

permanent deformation of keratin fibers

INVENTOR(S): Vic, Gabin; Livoreil, Aude; Samain, Henri

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 20 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

AB The invention relates to a cosmetic composition for the permanent deformation of keratinous fibers, in particular those of the hair, and composed of at least a nitrosonium salt.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1154307 HCAPLUS

DOCUMENT NUMBER: 142:79554

TITLE: Cosmetic composition containing a precursor of a thiyl

radical for the permanent waving of keratinous fibers

INVENTOR(S): Vic, Gabin; Livoreil, Aude; Samain, Henri

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

20041229 EP 2004-300403 EP 1491181 A2 20040628 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR FR 2856592 A1 20041231 FR 2003-50267 20030627 PRIORITY APPLN. INFO.: FR 2003-50267 A 20030627 MARPAT 142:79554 OTHER SOURCE(S): The invention involves a cosmetic composition intended for the permanent waving of keratinous fibers, particularly hairs, and composed of at least one thiyl radical. L26 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN 2004:995898 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 141:415602 Dithiols in a hair-perming composition TITLE: Samain, Henri; Genain, Gilles; Livoreil, Aude INVENTOR (S): ; Vic, Gabin L'oreal, Fr. PATENT ASSIGNEE(S): PCT Int. Appl., 23 pp. SOURCE: CODEN: PIXXD2 Patent DOCUMENT TYPE: French LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. PATENT NO. KIND DATE DATE ------------------------WO 2004098488 A2 20041118 WO 2004-FR1071 20040504 A3 WO 2004098488 20041229 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG FR 2854568 A1 20041112 FR 2003-5496 20030506 FR 2003-5496 PRIORITY APPLN. INFO.: A 20030506 US 2003-477366P P 20030611 MARPAT 141:415602 OTHER SOURCE(S): The invention relates to the use of particular dithiols in a hair-perming composition The invention also relates to a hair-perming method employing the dithiols as well as cosmetic compns. containing at least one of the dithiols and at least 1 compound selected from among surfactants and nonionic, anionic, cationic, amphoteric or zwitterionic polymers or cosmetic compns. containing specific dithiols. Thus, a formulation contained a dithiol 20.83, ammonia qs to pH 7, and water qs to 100 g. L26 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN 2004:992715 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 141:415631 TITLE: Processes for removing makeup and reapplying it to hair after receptor ligand treatment INVENTOR(S): Vic, Gabin; Livoreil, Aude; Bernard, Bruno PATENT ASSIGNEE(S): L'oreal, Fr. SOURCE: Fr. Demande, 14 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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KIND DATE APPLICATION NO.
PATENT NO.
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                         20041119 FR 2003-5775 20030514
20041125 WO 2004-FR1090 20040506
FR 2854796
                   A1
                         20041125 WO 2004-FR1090
WO 2004100911
                  A1
   W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
       CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
       GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
       LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
       NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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   RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
       AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
       EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
       SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
       SN, TD, TG
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PRIORITY APPLN. INFO.:

FR 2003-5775 A 20030514

AB Make-ups are removed from keratin fibers and reapplied to the hair after a treatment of the fibers by ligand receptor system and. amino acids or salts. The hair is treated with biotin (500  $\mu g/mL$ ) in a phosphate buffer.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:962899 HCAPLUS

DOCUMENT NUMBER: 141:415614

TITLE: Use of dithiols in a composition for permanent waving

of hair

INVENTOR(S): Samain, Henri; Genain, Gilles; Livoreil, Aude

; Vic, Gabin

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 28 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PAT	PATENT NO.					D	DATE			APPL	ICAT	ION 1	NO.			ATE	
FR	2854	568			A1	-	2004	1112		FR 2	003-	5496				0030	
WO	2004	0984	88		A2		2004	1118	1	WO 2	004-	FR10	71		2	0040	504
WO	2004	0984	88		A3		2004	1229									
	W:	ΑĒ,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	TG												•	
PRIORITY	IORITY APPLN. INFO.:									FR 2	003-	5496		I	A 20	0030	506

Page 200

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Pryor 09_666463
                        KIND
                              DATE
                                          APPLICATION NO.
                                                                DATE
    PATENT NO.
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                              20040701 WO 2003-FR3698
    WO 2004054527
                        A1
                                                                20031212
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
            NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
            TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
            ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
            TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    FR 2848428
                        A1
                              20040618
                                        FR 2002-15860 20021213
    EP 1572139
                        A1
                              20050914
                                         EP 2003-813178
                                                               20031212
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO.:
                                          FR 2002-15860 A 20021213
                                          US 2003-448112P
                                                            P 20030220
                                          WO 2003-FR3698
                                                            W 20031212
    The invention concerns a cosmetic composition comprising a cosmetic active
AB
    agent and one photodimerizable compound enabling a material deposit to be
    provided on the keratin materials, which are resistant to washing. The
    location is precisely controlled and is capable of providing long-lasting
    cosmetic properties to the keratin materials. Thus, an aqueous dispersion
    containing poly(vinyl acetate) partially saponified and carrying stilbazolium
    groups was adsorbed on poly(vinyl acetate) particles. A formulation
    comprised the above dispersion 11.25, Skinotan S10 (a Dimethicone
    copolyol) 0.5, and water qs to 100 q.
REFERENCE COUNT:
                        8
                              THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L26 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
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ACCESSION NUMBER: 2004:492299 HCAPLUS

DOCUMENT NUMBER: 141:59210

TITLE: Cosmetic compositions comprising a photodimerizable

compound

Samain, Henri; Vic, Gabin; Livoreil, Aude; INVENTOR (S):

Giroud, Franck

L'Oreal, Fr. PATENT ASSIGNEE(S):

SOURCE: Fr. Demande, 41 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.		KIN	D DAT	E		APPL	ICAT	ION 1	. 00		D	ATE	
FR 2848428		A1		40618		FR 2			-			0021	
WO 2004054	527	A1	200	40701		WO 2	003-	FR36	98		20	0031	212
W: AE	AG, A	AL, AM,	AT, AU	, AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
CN	co, c	CR, CU,	CZ, DE	, DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
GE	GH, C	GM, HR,	HU, II	, IL,	IN,	IS,	JP,	ΚE,	KG,	KΡ,	KR,	ΚZ,	LC,
LK	LR, I	LS, LT,	LU, LV	, MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,
NZ	OM, I	PG, PH,	PL, PI	, RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,
TM	TN, T	rr, TT,	TZ, UA	, UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	zw	
RW: BW	GH, C	GM, KE,	LS, MW	, MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,
BY	KG, F	KZ, MD,	RU, TJ	, TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,
ES	FI, F	FR, GB,	GR, HU	, IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,

US 2003-477366P P 20030611

OTHER SOURCE(S): MARPAT 141:415614

The use of dithiols in hair compns. for permanent deformation of the hair is disclosed. A process for permanent deformation of the hair implementing these dithiols and at least a surfactant and nonionic, anionic, cationic, amphoteric or zwitterionic polymers also is disclosed. A reducing lotion contained N,N'-dimethyl-N,N'-di (mercaptoacetyl) hydrazine 20.83, ammonia q.s. pH = 7, and water q.s. 100 g.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:960036 HCAPLUS

DOCUMENT NUMBER: 141:400482

TITLE: Alkaline straightening of the hair in the presence of

a hydrosoluble polymer having a high molecular weight

INVENTOR(S): Samain, Henri; Livoreil, Aude

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 1475075	A1 20041110	EP 2004-291136	20040504
		GB, GR, IT, LI, LU, NL	
IE, SI, LT,	LV, FI, RO, MK,	CY, AL, TR, BG, CZ, EE	, HU, PL, SK, HR
FR 2854567	A1 20041112	FR 2003-5451	20030505
US 2004265256	A1 20041230	US 2004-837642	20040504
PRIORITY APPLN. INFO.:		FR 2003-5451	A 20030505
		US 2003-477347P	P 20030611

OTHER SOURCE(S): MARPAT 141:400482

AB Hair straightener prepns. contain an alkaline straightening composition and a hydrosol. polymer having a high mol. weight The two composition are applied simultaneously or successively on the hair. A hair straightener prepns. contained sodium hydroxide 1.99, Ultimer TX-11415 6.65, and water q.s. 100 g. The composition was applied on the hair for 20 min and then, washed with water and dried. The composition produced more porosity in the hair than the control composition containing no hydrosol. polymer.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:531322 HCAPLUS

DOCUMENT NUMBER: 141:76400

TITLE: Cosmetic compositions comprising a photodimerizable

compound for treating keratin materials

INVENTOR(S): Samain, Henri; Vic, Gabin; Livoreil, Aude;

Giroud, Franck

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG A1 20050914 EP 2003-813178 20031212 EP 1572139 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK PRIORITY APPLN. INFO.: FR 2002-15860 A 20021213 US 2003-448112P P 20030220 W 20031212 WO 2003-FR3698 MARPAT 141:59210 OTHER SOURCE(S): A cosmetic composition contains a compound with photodimerizable groups. Thus, a composition contained a dispersion of poly(vinyl acetate) (PVA) containing stilbazolium groups adsorbed on PVA particles 11.25, Dimethicone copolyol (Skinostan S10) 0.5, and water qs to 100 g. 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L26 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN 2004:446883 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 140:428669 TITLE: Cosmetic hair treatment process for imparting enduring cosmetic properties to hair Vic, Gabin; Livoreil, Aude; Daubresse, INVENTOR(S): Nicolas L'Oreal, Fr. PATENT ASSIGNEE(S): Eur. Pat. Appl., 11 pp. SOURCE: CODEN: EPXXDW DOCUMENT TYPE: Patent French LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE ----\_\_\_\_\_\_ ----------A1 20040602 EP 2003-292930 EP 1424061 20031126 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK FR 2847806 20040604 FR 2002-15076 A1 20021129 US 2004156803 **A1** 20040812 US 2003-721106 20031126 JP 2004182731 A2 20040702 JP 2003-401539 20031201 PRIORITY APPLN. INFO.: FR 2002-15076 A 20021129 US 2002-434665P P 20021220 A process for treatment of hair comprises a non-reducing step of hair AΒ activation and a second step of applying a cosmetic composition able to form a covalent bond with the activated hair. A solution containing polyethyleneimine 10, 36% HCl qs to pH 8, and water qs 100 g was applied on the hair and kept at 60° for 30 min., then a solution containing Reactive Blue-4 dye 5, and water qs 100 g was applied onto the hair and kept at 30° for another 30 min. The hair was then washed with water and dried to obtain the desired color. L26 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2004:249283 HCAPLUS DOCUMENT NUMBER: 140:275720 Cosmetic composition containing a ligand-exogenous TITLE: receptor system adsorbed or fixed in a covalent way to keratinic material and treatment of the hair using this composition or its components INVENTOR (S): Vic, Gabin; Livoreil, Aude; Bernard, Bruno PATENT ASSIGNEE(S): L'oreal, Fr.

Fr. Demande, 55 pp.

SOURCE:

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844712	A1	20040326	FR 2002-11782	20020924
JP 2005023016	A2	20050127	JP 2003-189618	20030701
BR 2003003867	Α	20040908	BR 2003-3867	20030922
EP 1402880	A1	20040331	EP 2003-292330	20030923
R: AT, BE, CH,	DE, DK	, ES, FR, GI	B, GR, IT, LI, LU,	NL, SE, MC, PT,
IE, SI, LT,	LV, FI	, RO, MK, C	Y, AL, TR, BG, CZ,	EE, HU, SK
US 2004208843	<b>A</b> 1	20041021	US 2003-667435	20030923
JP 2004115518	A2	20040415	JP 2003-331415	20030924
CN 1494893	Α	20040512	CN 2003-159754	20030924
PRIORITY APPLN. INFO.:			FR 2002-11782	A 20020924

Cosmetic compns. contain a cosmetic agent fixed in a covalent way to one of both of (a) a compound and/or a (b) sequestering agent of this compound The invention also relates to processes of treatment of the keratinous matters with these compns. A solution of antifluorescein isothiocyanate (anti-FITC) was applied on the hair, then washed with Tween-20. The treated hair was then, put in a solution of FITC-dextran for two hours, then it was washed. Anal. of the hair showed that dextran was deposited on the hair while there was no dextran on the hair which was not treated with anti-FITC.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2003:895807 HCAPLUS

DOCUMENT NUMBER:

139:369378

TITLE:

Cosmetic compositions containing photoactivated

diazirines

INVENTOR(S):

Vic, Gabin; Livoreil, Aude

PATENT ASSIGNEE(S):

L'oreal, Fr.

SOURCE:

Fr. Demande, 21 pp.

CODEN: FRXXBL

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.	KIND	DATE	APPLICATION NO.	DATE
FR 283	9446	A1	20031114	FR 2002-5863	20020513
EP 136	2851	A1	20031119	EP 2003-291041	20030429
R:	AT, BE, CH	, DE, DE	K, ES, FR,	GB, GR, IT, LI, LU, N	L, SE, MC, PT,
	IE, SI, LT	', LV, F	I, RO, MK,	CY, AL, TR, BG, CZ, E	E, HU, SK
JP 200	3335638	A2	20031125	JP 2003-134790	20030513
US 200	4043046	A1	20040304	US 2003-436050	20030513
US 200	5118207	A9	20050602		
PRIORITY AP	PLN. INFO.:			FR 2002-5863	A 20020513
				US 2002-386571P	P 20020607

OTHER SOURCE(S): MARPAT 139:369378

A cosmetic composition contains at least a diazirine covalently bound to a cosmetic ingredient. Thus, Jeffamine M1000 was allowed to react with a diazirine derivative The compound was applied on natural hair and the hair was irradiated at 360 nm for 30 min.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:837576 HCAPLUS

DOCUMENT NUMBER: 139:327947

TITLE: Hair compositions containing exogenous ligand-receptor

system

INVENTOR(S): Vic, Gabin; Livoreil, Aude; Bernard, Bruno

PATENT ASSIGNEE(S): L'oreal, Fr. SOURCE: Fr. Demande, 52 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

I	ra9	ENT	NO.			KIN	D	DATE		A	PP!	LICA	CION	NO.			DA'	ΓE	
-							-			-									<del>-</del>
F	FR	2838	640			<b>A1</b>		2003	1024	F	R 2	2002-	4952				200	0204	119
(	CA	2424	531			AA		2003	1019	C	A :	2003-	2424	531			200	0304	111
F	ΞP	1358	867			<b>A1</b>		2003	1105	E	P :	2003-	2909	39			200	0304	116
		R:	ΑT,	BE,	CH,	DE,	DK	, ES,	FR,	GB, G	GR.	, IT,	LI,	LU,	NL,	SE	, 1	MC,	PT,
			ΙE,	SI,	LT,	LV,	FI	, RO,	MK,	CY, Z	AL.	, TR	BG,	CZ,	EE,	HU	, ,	SK	
. I	3R	2003	0012	76		Α		2004	0817	B	2	2003-	1276				20	0304	117
(	CN	1451	370			Α		2003	1029	CI	V 2	2003-	1225	28			200	0304	118
Ċ	JΡ	2004	0023	98		A2		2004	0108	J	P 2	2003	1157	23			200	0304	121
J	JS	2004	0429	93		A1		2004	0304	U	3 2	2003-	4192	57			20	0304	121
PRIOR	ΙΤΥ	APP	LN.	INFO	. :					F	R :	2002-	4952			Α	20	0204	119
										U	3 2	2002-	3965	81P		P	200	0207	718

OTHER SOURCE(S): MARPAT 139:327947

AB Cosmetic compns. contain biotin and/or a sequestering agent, capable of forming complexes with biotin. The present invention relates also to a process of treatment of the hair containing the above composition Thus, TFP-PEG-biotin compound was fixed on the hair surface by using the

avidin-peroxidase complex. The above compound was resistant to shampooing.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:798404 HCAPLUS

DOCUMENT NUMBER: 139:311933

TITLE: Organically modified metal particles for the treatment

of human hair

INVENTOR(S): Vic, Gabin; Livoreil, Aude; Giroud, Franck

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 29 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2838052	A1	20031010	FR 2002-4354	20020408
US 2004010864	A1	20040122	US 2003-393924	20030324
BR 2003001010	Α	20040817	BR 2003-1010	20030404
EP 1352634	A1	20031015	EP 2003-290859	20030407
R: AT, BE, CH,	DE, DK	, ES, FR, GE	B, GR, IT, LI, LU, NL,	SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK 20031021 JP 2003-104224 JP 2003300844 A2 20030408 20040512 CN 2003-110321 CN 1494894 Α 20030408 PRIORITY APPLN. INFO.: FR 2002-4354 A 20020408 US 2002-396581P P 20020718

AB The invention relates to the use of a suspension of organically modified metallic nanoparticles carrying on their surface a monolayer obtained from organosulfur compds. for the coloring and/or the treatment of human hair. Nanoparticles of gold modified by mercaptosuccinic acid were obtained by the treatment of HAuCl4.3H2O with mercaptosuccinic acid in the presence of NaBH4 in aqueous MeOH solution These nanoparticles were adsorbed on white hair fibers.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:798402 HCAPLUS

DOCUMENT NUMBER: 139:311931

TITLE: Metal coating of hair fibers for cosmetics INVENTOR(S): Vic, Gabin; Livoreil, Aude; Giroud, Franck

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 18 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2838050	A1	20031010	FR 2002-4352	20020408
CN 1449737	Α	20031022	CN 2003-108449	20030331
BR 2003000873	Α	20040817	BR 2003-873	20030403
EP 1352630	A2	20031015	EP 2003-290860	20030407
EP 1352630	A3	20040324		
R: AT, BE, CH,	DE, DK	, ES, FR, GB	B, GR, IT, LI, LU, NL,	SE, MC, PT,
IE, SI, LT,	LV, FI	, RO, MK, CY	, AL, TR, BG, CZ, EE,	HU, SK
US 2003223944	A1	20031204	US 2003-407911	20030407
JP 2003300840	A2	20031021	JP 2003-104420	20030408
PRIORITY APPLN. INFO.:			FR 2002-4352	A 20020408
			US 2002-372455P	P 20020416

AB The invention relates to a treatment process which confers cosmetic properties on hair fibers. The process consists of treating the fibers with a metal salt in the presence of a reducing agent, directly on the fiber to form the corresponding free metal. Thus, a lock of hair after being shampooed, was dried and an aqueous solution of AgNO3 was applied onto the

hair. After the addition of NaBH4, the natural pigmented hair was dark, with metallic brilliance reflected on it.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:659849 HCAPLUS

DOCUMENT NUMBER: 139:169001

TITLE: Use in cosmetics of stable aqueous dispersions of core-shell-type particles with reactive silyl groups

INVENTOR(S): Rollat, Isabelle; Livoreil, Aude; Vic, Gabin

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 15 pp.

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WO 2003059299
                               20030724
                                         WO 2002-FR4595
                         A1
                                                                 20021231
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
            UG, US, UZ, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
            CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1461002
                        A1
                            20040929 EP 2002-799133
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
PRIORITY APPLN. INFO.:
                                          FR 2001-17074
                                                           A 20011231
                                          WO 2002-FR4595
                                                              W 20021231
OTHER SOURCE(S):
                       MARPAT 139:73721
    Cosmetic compns. comprise a biotin derivative and/or a complexing agent for
    hair dyeing. Hair dyes were prepared containing avidin-biotin.
L26 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
                        2003:475492 HCAPLUS
DOCUMENT NUMBER:
                        139:41436
TITLE:
                        Cosmetic hair preparation forming soft coating
                        comprising a polymer having non-silicone skeleton and
                        reactive group
INVENTOR(S):
                        Samain, Henri; Rollat, Isabelle; Giroud, Franck;
                        Mougin, Nathalie; Livoreil, Aude
PATENT ASSIGNEE(S):
                        L'Oreal, Fr.
                        Fr. Demande, 29 pp.
SOURCE:
                        CODEN: FRXXBL
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        French
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                         APPLICATION NO.
    PATENT NO.
                        KIND DATE
                                                                 DATE
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                              _____
                                         _____
    FR 2833600
                        A1
                               20030620
                                         FR 2001-16384
                                                                 20011218
    FR 2833600
                        B1 20040813
A1 20030625
                        B1
                               20040813
    EP 1321125
                                         EP 2002-292957
                                                                 20021129
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
                                        CN 2002-140020
    CN 1448125 A
                               20031015
                                                                20021217
    JP 2003192547
                        A2
                               20030709
                                         JP 2002-367351
                                                                 20021218
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08

US 2002-321361 US 2003165450 A1 20030904 20021218 BR 2002-5588 BR 2002005588 Α 20040803 20021218 A 20011218 PRIORITY APPLN. INFO.: FR 2001-16384 A cosmetic hair preparation contains a non-silicone polymer, with reactive chemical functions, ready to form a soft coating on the hair. A hair composition

contained 10% poly(glycidyl methacrylate) 20, ethylenediamine 5, 22% ammonia q.s. pH = 9, methylethyl ketone 20, and water q.s. 100 g.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:475472 HCAPLUS

DOCUMENT NUMBER: 139:57626

TITLE: Cosmetic compositions comprising polymers having

CODEN: FRXXBL

DOCUMENT TYPE: Patent French LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PAT	CENT 1	KIN	)	DATE		APPLICATION NO.						DATE					
							-								- <b>-</b>	-		
	FR	2836	041					2003			FR 20	002-2	2187			2	0020	221
	FR	2836	041			В1		2004	0521									
	WO	2003	0702	05		A1		2003	0828	1	WO 2	003-1	FR49	0		2	0030	214
	WO	2003	0702	05		C1		2004	0506									
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
11			GM.	HR.	HU.	TD.	TL.	TN.	TS.	JP.	KE.	KG.	KP.	KR.	KZ.	LC.	LK.	LR.
<i></i>	٦,		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
			PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
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1		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
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	EP	1478	•	•	•	•	•	2004						•	•			
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										1	WO 2	003-1	FR49	0	1	N 2	0030:	214
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The present invention relates to the use in cosmetic, and in particular AΒ for the treatment of human keratinous fibers, of an aqueous dispersion of particles of the core/envelope-type formed from an envelope containing insol. acrylic polymers in water, and of a core containing compds. with reactive silyl functions. A hair preparation contained Sanmol EW102 10, water 100, and ammonium hydroxide ph 8.5%. The particle size after 2 mo storage at 45° was 149 nm.

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN 2003:516837 HCAPLUS ACCESSION NUMBER:

3

DOCUMENT NUMBER: 139:73721

Cosmetic compositions containing a active cosmetic TITLE: agent and an exogenous hair ligand-receptor system and

a method of treatment of the hair using these

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

compositions

Vic, Gabin; Livoreil, Aude; Bernard, Bruno INVENTOR(S):

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: Fr. Demande, 44 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

REFERENCE COUNT:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2834209	A1	20030704	FR 2001-17074	20011231
FR 2834209	B1	20040423		
US 2003161803	A1	20030828	US 2002-330481	20021230

complementary chemical groups

Samain, Henri; Rollat, Isabelle; Vic, Gabin; INVENTOR(S):

Livoreil, Aude

PATENT ASSIGNEE(S):

SOURCE:

L'Oreal, Fr. Fr. Demande, 24 pp.

CODEN: FRXXBL

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PAT	ENT 1	NO.			KINI	)	DATE		API	LICAT	'ION	NO.		D	ATE	
		·		- <b></b> -			-										
	FR	2833	487			A1		2003	0620	FR	2001-	1638	7		20	0011	218
	FR	2833	487			В1		2004	0827								
	ΕP	1321	126			A1		2003	0625	EP	2002-	2929	58		20	0021	129
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			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY, AI	, TR,	BG,	CZ,	EE,	SK		
	CN	1426	772			Α		2003	0702	CN	2002-	1518	70		20	0021	217
	JP	2003	1925	42		A2		2003	0709	JP	2002-	367.3	52		. 20	0021	218
	US	2003	1431	75		A1		2003	0731	<b>413</b>	2002-	3213	555		.20	0021	218
	BR	2002	0071	47		Α		2003	0930	BR	2002-	7147			. 20	0021	218
) [	የ ተጥነ	APP	LN.	TNFO	. :					FR	2001-	1638	7	7	1 2	0011	218

PRIORITY APPLN. INFO.: Cosmetic compns. contain at least two polymers with complementary chemical groups ready to form a coating on the keratinous fibers, and in particular on hair. A hair preparation contained starbust PAMAM dendrimer 50, and 5% Gantrez S-97BF 50 g. The preparation was applied on the hair and left to dry,

then kept for 2 h at 100°. The composition remained on the hair even after 10 washing with shampoo.

REFERENCE COUNT:

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 23 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

11

ACCESSION NUMBER:

2003:475471 HCAPLUS

DOCUMENT NUMBER:

139:57625

TITLE:

Cosmetic composition forming a tackant coating

comprising a polymer having a non-silicone skeleton

and reactive groups

INVENTOR(S):

Samain, Henri; Rollat, Isabelle; Giroud, Franck;

Mougin, Nathalie; Livoreil, Aude

PATENT ASSIGNEE(S):

SOURCE:

L'Oreal, Fr.

Fr. Demande, 33 pp.

CODEN: FRXXBL

DOCUMENT TYPE: LANGUAGE:

Patent French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT 1	NO.			KIN	) · I	DATE		;	APPL:	ICAT	ION I	NO.		D	ATE	
<del>-</del>		<b>-</b>			-									-		
FR 2833	486			A1	:	2003	0620		FR 20	001-	1638	6		2	0011	218
FR 2833	486			B1	:	2004	0820									
WO 2003	05337	79		A1	:	2003	0703	1	WO 2	002-	FR41	57		2	0021	203
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	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JΡ,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw						
RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,

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KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                          EP 2002-805358
                                                                   20021203
     EP 1458336
                          Α1
                                20040922
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
                                            V$ 2002-321359 ✓
     US 2003157136
                         A1
                                20030821
                                                                   20021218
                                            FR 2001-16386
PRIORITY APPLN. INFO .:
                                                                A 20011218
                                            WO 2002-FR4157
                                                                W 20021203
     A cosmetic hair preparation contains a non-silicone polymer, with reactive
AB
     chemical functions, ready to form a tackant coating on the hair. A polymer
     was prepared by the reaction of Me itaconate, diethylene triamine, and
     epichlorohydrin. A hair composition contained above polymer 5,
     monoethanolamine 1, and water q.s. 100 g.
REFERENCE COUNT:
                         8
                               THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L26 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
                         2003:475470 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         139:41433
                         Cosmetic hair preparation forming a soft coating
TITLE:
                         comprising a polymer having a non-silicone skeleton
                         and a reactive group
INVENTOR(S):
                         Samain, Henri; Rollat, Isabelle; Giroud, Franck;
                         Mougin, Nathalie; Livoreil, Aude
PATENT ASSIGNEE(S):
                         L'Oreal, Fr.
                         Fr. Demande, 28 pp.
SOURCE:
                         CODEN: FRXXBL
DOCUMENT TYPE:
                         Patent
                         French
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                        KIND
                                DATE
                                          APPLICATION NO.
                                                                   DATE
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                                20030620
                                           FR 2001-16385
                                                                   20011218
     FR 2833485
                         A1
     FR 2833485
                         В1
                                20050211
    WO 2003053378
                                20030703
                                            WO 2002-FR4156
                                                                   20021203
                         A2
     WO 2003053378
                         Α3
                                20040122
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1458335
                         A2
                                20040922
                                          EP 2002-801095
                                                                   20021203
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
                                20031002 (<u>US</u> 2002-321450 )
     US 2003185781
                         A1
PRIORITY APPLN. INFO .:
                                            FR 2001-16385
                                                                A 20011218
                                            WO 2002-FR4156
                                                                W 20021203
```

AB A cosmetic hair preparation contains a non-silicone polymer, with reactive chemical functions, ready to form a soft coating on the hair. A polymer was prepared by the reaction of adipic acid, diethylene triamine, piperazine, and epichlorohydrin. A hair composition contained above polymer 5, monoethanolamine 1, and water q.s. 100 g.

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 3 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L26 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN 2003:335835 HCAPLUS ACCESSION NUMBER: 138:358166 DOCUMENT NUMBER: Photo-activable compound for use is cosmetics TITLE: Vic, Gabin; Livoreil, Aude INVENTOR(S): L'oreal, Fr. PATENT ASSIGNEE(S): Fr. Demande, 31 pp. SOURCE: CODEN: FRXXBL

Patent DOCUMENT TYPE: LANGUAGE: French FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	TENT	NO.			KIN	)	DATE		i	APPL	ICAT:	ION I	NO.		D	ATE	
			<b></b>			-					- <b></b> -						
FR	2831	534			A1		2003	0502		FR 2	001-	1397	0		20	0011	029
FR	2831	534			B1		2004	0130									
WO	2003	03783	30		A2		2003	0508	1	WO 2	002-3	FR36	32		2	0021	023
WO	2003	0378	30		А3		2003	1016					•				
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		CO,	CR,	CU,	CZ,	ĎΕ,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KΡ,	KR,	ΚZ,	LC,	LK,	LR,
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	RW:	GH.	GM,	KE.	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	AZ,	BY,
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.тп	2005															0021	023
UF	2003	1122	70		λ1		2003	0517		IIS 2	002-	2797	57	>		0021	
					AT		2003	0019		FR 2					_	0011	
PRIORIT	Y APP	ъΝ.	TNFO	. :									-		-		
										WO 2	002-	FR36	32		w 2	0021	023

MARPAT 138:358166 OTHER SOURCE(S):

Photo-activable compds. for use in cosmetics are claimed. Photo-activable ovalbumin was prepared by the reaction of ovlabumin with

N-hydroxysulfosuccinimidyl-4-azidobenzoate. A composition containing

photo-activable ovalbumin and fluorescent dextran was prepared

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 1 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

2002:946071 · HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 138:28948

Cosmetic composition forming after application of a TITLE:

supramolecular polymer

INVENTOR(S): Mougin, Nathalie; Livoreil, Aude; Mondet,

Jean

PATENT ASSIGNEE(S): L'oreal, Fr.

PCT Int. Appl., 82 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent · LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

#### PATENT INFORMATION:

	PATENT NO.						)	DATE APPLICATION NO.						DATE				
	WO	20020	 0983'	 7 <b>7</b>		A1 20021212								<b>-</b> -	2	0020	 607	
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI.	GB,	GD.	GE,	GH.
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									MG,									
									SG,									
									ZA,									
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									GB,									
									GA,	•	•		•	•	•	•		•
	FR	2825			•	A1	•		1213	•		•	•			•	0010	
	FR	2825	628			В1		2004	0319									
	EΡ	1392	222			A1		2004	0303	]	EP 20	002-	7475	20		2	0020	607
									FR,									
									MK,				•	•	•	•	•	•
	JP	2005			•		•			•			5014	19		2	0020	607
	US	2004	1613	94		A1		2004	0819	/	JS 20	003-	1797	16>		2	0031	205
PRIO		APP															0010	
															7		0020	
	_,																	

AB The invention concerns a cosmetic composition for care and/or treatment and/or make-up of keratinous materials, comprising, in a physiol. acceptable medium, an efficient amount of at least a linear, branched or cyclic, or dendritic polymer, comprising: a polymeric skeleton including at least two repeat units, and at least two functional groups (A) fixed on the polymeric skeleton and capable of binding with one or several partner junction groups, of identical or different chemical type, each matching of two functional groups involving at least three H bridges. Preparation of a ureido pyrimidone polydimethylsiloxane and a lipstick containing this polymer is disclosed.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:944461 HCAPLUS

DOCUMENT NUMBER: 138:8260

TITLE: Use of a polar additive in a cosmetic composition

containing a structured liquid oil phase by at least one organogelator to give a thixotropic character

INVENTOR(S): Livoreil, Aude; Baqhdadli, Nawel

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 1264589	A1 20021211	EP 2002-291423	20020607
R: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IT, LI, LU, NL,	SE, MC, PT,
IE, SI, LT,	LV, FI, RO, MK,	CY, AL, TR	
FR 2825618	A1 20021213	FR 2001-7474	20010607
JP 2002370926	A2 20021224	JP 2002-167454	20020607
US 2003091520	A1 20030515	US 2002-163509	20020607

PRIORITY APPLN. INFO.: FR 2001-7474 A 20010607 A polar additive having a polarity parameter  $\delta a \geq 7.0$ (j/cm3)1/2 is used in a cosmetic composition containing a liquid oil phase containing an apolar or weakly polar oil having a polarity parameter  $\delta a \leq$ 7.0 (j/cm3)1/2 structured by at least one organogelator to give a thixotropic character. Formulation of a cosmetic composition containing octyldodecanol and 2-ethylhexyl palmitate is disclosed. THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L26 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN 2002:69335 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 136:123393 TITLE: Cosmetic or pharmaceutical solid composition comprising bis-acyl-amides Livoreil, Aude; Genard, Sylvie INVENTOR(S): PATENT ASSIGNEE(S): L'Oreal, Fr. Eur. Pat. Appl., 21 pp. SOURCE: CODEN: EPXXDW DOCUMENT TYPE: Patent LANGUAGE: French FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: DATE APPLICATION NO. DATE PATENT NO. KIND Al 20020123 EP 2001-401905 20010716 \_\_\_\_\_\_ EP 1174110 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO FR 2811552 FR 2000-9317 -A1 20020118 FR 2811552 B1 20021227 CA 2382085 AA20020124 CA 2001-2382085 WO 2001-FR2306 WO 2002005763 A1 20020124 2002005763

A1 20020124 WO 2001-FR2306 20010716
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 20020430 BR 2001-7027 20031227 RU 2002-110122 20040205 JP 2002-511697 20040318 AU 2001-76457 BR 2001007027 Α 20010716 RU 2219899 C1 20010716 JP 2004503575 T2 20010716 AU 771283 B2 20010716 A5 A AU 2001076457 20020130 ZA 2002000993 20020816 ZA 2002-993 20020205 A1 US 2002150602 20021017 US 2002-88296 20020410 US 2003129211 A9 20030710 US 6726915 20040427 A 20000717 PRIORITY APPLN. INFO.: FR 2000-9317 W 20010716 WO 2001-FR2306 OTHER SOURCE(S): MARPAT 136:123393 Cosmetic or pharmaceutical solid compns. comprising an oily phase and a bis-acyl-amide RCONH-A-NHCOR' (R, R' = H, hydrocarbon chain; A = hydrocarbon chain) are claimed. A transparent cosmetic stick contained trans-N,N'-bis(dodecanoyl)-1,2-diaminocyclohexane 220 mg, and tridecyl trimellitate fatty ester 10 mL.

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

3

REFERENCE COUNT:

### RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:424432 HCAPLUS

DOCUMENT NUMBER: 131:208068

TITLE: Transition metal-containing Catenanes and rotaxanes:

control of electronic and molecular motions

Chambron I.C. Sayvage I.P. Collin I.P.

AUTHOR(S): Chambron, J.-C.; Sauvage, J.-P.; Collin, J.-P.; Gavina, P.; Heitz, V.; Linke, M.; Livoreil, A.

CORPORATE SOURCE: Laboratoire de Chimie Organo-Minerale, CNRS-UMR 7513,

Universite Louis Pasteur, Institut Le Bel, Strasbourg,

67070, Fr.

SOURCE: NATO ASI Series, Series C: Mathematical and Physical

Sciences (1999), 527(Supramolecular Science: Where It

Is and Where It Is Going), 23-28 CODEN: NSCSDW; ISSN: 0258-2023 Kluwer Academic Publishers

PUBLISHER: Kluwer Academic Publisher DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 18 refs. describes development of functional catenanes and rotaxanes, that is mols. responding to external stimuli, like injection or removal of electrons, light irradiation, and so on. Examples are rotaxanes and catenanes displaying electrochem.-triggered intramol. motions such as translation of the ring along the dumbbell axle, rotation of one ring within the other, or photochem.-induced electron transfer from Zn(II)-porphyrin stoppers (electron donors in the excited state) to a Au(III) porphyrin electron acceptor appended to the ring component.

L26 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:798559 HCAPLUS

DOCUMENT NUMBER: 127:365393

TITLE: Electrochemically and Photochemically Driven Ring

Motions in a Disymmetrical Copper [2]-Catenate

AUTHOR(S): Livoreil, Aude; Sauvage, Jean-Pierre;

Armaroli, Nicola; Balzani, Vincenzo; Flamigni, Lucia;

Ventura, Barbara

CORPORATE SOURCE: Laboratoire de Chimie Organo-Minerale URA 422 du CNRS

Institut Le Bel, Universite Louis Pasteur, Strasbourg,

67070, Fr.

SOURCE: Journal of the American Chemical Society (1997),

119(50), 12114-12124

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

By applying the three-dimensional template effect of copper(I), previously used for making various interlocking ring systems, a new disym.

[2]-catenate was made which consists of two different interlocking rings. One ring contains a 2,9-diphenyl-1,10-phenanthroline (dpp) unit whereas the other cycle incorporates both a dpp motif and a 2,2',6',2''-terpyridine (terpy) fragment, the coordination site of these two chelates pointing toward the inside of the ring. Depending on the oxidation state of the central metal (Cu(I) or Cu(II)), and thus on its preferred coordination number, two distinct situations were observed With monovalent copper, the two dpp units interact with the metal and the terpy fragment remains free, at the outside of the mol. By contrast, when the catenate is complexed to divalent copper, the terpy motif is bonded to the metal and it is now a dpp ligand which lies at the periphery of the complex. This dual coordination mode leads to dramatically different mol. shapes and properties for both forms. The mol. motion which interconverts the

four- and the five-coordinate complexes can be triggered chemical, electrochem., or photochem. by changing the oxidation state of the copper center (II/I). The process was studied by electrochem. and by UV-visible spectroscopy. Once the stable 4-coordinate copper(I) complex was oxidized to a thermodynamically unstable pseudo-tetrahedral copper(II) species, the rate of the gliding motion of the rings which will afford the stable 5-coordinate species (copper(II) coordinated to dpp and terpy) can be controlled at will. Under certain exptl. conditions, the changeover process is extremely slow (weeks), and the 5-coordinate complex is more or less frozen. By contrast, addition of a coordinating counterion to the medium (Cl-) enormously speeds up the rearrangement and leads to the thermodynamically stable 5-coordinate complex within minutes.

REFERENCE COUNT: 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:411312 HCAPLUS

TITLE: Study of recognition of amino-acids by a bis-porphyrinic transition metal complex

AUTHOR(S): Livoreil, A.; Hayashi, T.; Sauvage, J. P.;

Oqoshi, H.

CORPORATE SOURCE: Laboratory of Mineral-Organic Chemistry, Institut Le

Bel, Universite Louis Pasteur, Strasbourg, 67070, Fr.

SOURCE: Journal of Inorganic Biochemistry (1997), 67(1-4), 117

CODEN: JIBIDJ; ISSN: 0162-0134

PUBLISHER: Elsevier DOCUMENT TYPE: Journal

LANGUAGE: English

AB Unavailable

L26 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:197660 HCAPLUS

DOCUMENT NUMBER: 126:244977

TITLE: Switchable interlocked molecules, threaded complexes

and interlocking in crystals

AUTHOR(S): Amabilino, David B.; Dietrich-Buchecker, Christiane

O.; Livoreil, Aude; Perez-Garcia, Lluisa; Sauvage, Jean-Pierre; Stoddart, J. Fraser

CORPORATE SOURCE: Laboratoire Chimie Organo-Minerale, Institute Le Bel,

Strasbourg, 67070, Fr.

SOURCE: NATO ASI Series, Series C: Mathematical and Physical

Sciences (1996), 484 (Magnetism: A Supramolecular

Function), 65-83

CODEN: NSCSDW; ISSN: 0258-2023

PUBLISHER: Kluwer

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review, with .apprx.54 refs. The advantages of interlocking for creating switchable chemical systems is discussed and reviewed, and contrasted with intertwined threaded complexes. The possibilities for obtaining interlocked superstructures - which necessarily require control of three-dimensional assembly processes - in the solid state from catenane components is discussed, and crystalline interpenetrating networks are reviewed.

L26 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:197656 HCAPLUS

DOCUMENT NUMBER: 126:283946

TITLE: Rotaxanes and catenanes in action

AUTHOR(S): Chambron, J.-C.; Dietrich-Buchecker, C.O.; Harriman,

A.; Heitz, V.; Livoreil, A.; Sauvage, J.-P.

CORPORATE SOURCE: Laboratoire de Chimie Organo-Minerale, Faculte de

Chimie, UA 422 au CNRS, Universite Louis Pasteur,

Strasbourg, 67000, Fr.

SOURCE: NATO ASI Series, Series C: Mathematical and Physical

Sciences (1996), 484 (Magnetism: A Supramolecular

Function), 1-8

CODEN: NSCSDW; ISSN: 0258-2023

PUBLISHER: Kluwer

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB Not only are rotaxanes and catenanes aesthetically and topol. attractive mols., but they can also be used as functional systems, able to undergo electronic and mol. motions under the action of an external stimulus. Porphyrin-stoppered rotaxanes are functional models of the photosynthetic Reaction Center, leading to ultrafast interporphyrin electron transfer under light irradiation. The efficiency of the process strongly relies on the rotaxane nature of the compound, being mostly determined by the properties of

the

central transition metal complex. Different is the function of a nonsym. Cu catenate, consisting of a two-coordination site ring interlocked to a 1-chelate incorporating cycle. The oxidation state of the Cu center (I or II) entirely dets. the set of ligands coordinated to the metal. Oxidizing or reducing the central Cu atom thus induces a complete gliding motion of one cycle within the other. This process can be regarded as electrochem. triggered swinging of the Cu catenate. A review with 20 refs.

L26 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:85783 HCAPLUS

DOCUMENT NUMBER: 126:230651

TITLE: Changeover in a multimodal copper(II) catenate as

monitored by EPR spectroscopy

AUTHOR(S): Baumann, Frank; Livoreil, Aude; Kaim,

Wolfgang; Sauvage, Jean-Pierre

CORPORATE SOURCE: Institut fur anorganische Chemie, Universitate

Stuttgart, Stuttgart, D-70550, Germany

SOURCE: Chemical Communications (Cambridge) (1997), (1), 35-36

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

AB The electrochem. triggered rearrangement of a copper catenate was monitored by EPR spectroscopy; the initially generated tetrahedral copper(II) complex (with higher g-factor components and lower metal hyperfine splitting) is converted to a stable five-coordinate copper(II) species, within a few minutes at room temperature, in anhydrous MeCN.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 35 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:672994 HCAPLUS

DOCUMENT NUMBER: 126:25955

TITLE: Redox Control of the Ring-Gliding Motion in a

Cu-Complexed Catenane: A Process Involving Three

Distinct Geometries

AUTHOR(S): Cardenas, Diego J.; Livoreil, Aude; Sauvage,

Jean-Pierre

CORPORATE SOURCE: Faculte de Chimie, Universite Louis Pasteur,

Strasbourg, 67000, Fr.

SOURCE: Journal of the American Chemical Society (1996),

118(47), 11980-11981

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB A multimodal coordinating [2]-catenane was synthesized as well as its Cu complexes. The compound consists of two identical interlocking rings, each ring incorporating both a bidentate and a terdentate chelating unit. The thermodynamically stable Cu(I) complex is 4-coordinate whereas the divalent state is preferably 6-coordinate. Interconversion between the three possible coordination nos. (CN = 4, 5 or 6) implies gliding of one ring within the other. This process corresponds to a complete geometrical change-over and can be induced either electrochem. or using chemical redox agents.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 36 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:203094 HCAPLUS

DOCUMENT NUMBER: 124:316409

TITLE: A Switchable Hybrid [2]-Catenane Based on Transition

Metal Complexation and  $\pi\text{-Electron Donor-Acceptor}$ 

Interactions

AUTHOR(S): Amabilino, David B.; Dietrich-Buchecker, Christiane

O.; Livoreil, Aude; Perez-Garcia, Lluiesa; Sauvage, Jean-Pierre; Stoddart, J. Fraser

CORPORATE SOURCE: Institut Le Bel, Universite Louis Pasteur, Strasbourg,

678070, Fr.

SOURCE: Journal of the American Chemical Society (1996),

118(16), 3905-13

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

A bimodal [2]-catenane was synthesized via a Cu(I) templated synthesis. The compound contains both a transition metal coordination site and a set of  $\pi$ -electron rich and  $\pi$ -electron deficient aromatic units suitable for the formation of acceptor-donor complexes. Each constituent ring is thus different from the other, and the organic backbone can adopt two favored contrasting orientations by circumrotation of one ring within the other: (i) in the metal complex mode, each dpp unit (dpp = 2,9-diphenyl-1,10phenanthroline) is entwined about the other, while a cationic species is complexed in the coordination site thus created; (ii) in the organic  $\pi$ -electron acceptor-donor complex mode, the dpp fragments are remote from one another, and the  $\pi$ -electron rich and  $\pi$ -electron deficient units stack to form a complex. The conversion of one binding mode to the other implies complete topog. rearrangement of the mol. It can be triggered by adding or removing the cation center (Cu+, Li+, or H+), bonded to the dpp-containing complexing site. This switching process can be easily monitored by 1H NMR, since it involves drastic relative orientational changes. It can also be evidenced by electronic spectroscopy. In particular, the proton-driven rearrangement reactions lead to significant changes in the absorption spectrum, which correspond to the appearance (by deprotonation) and disappearance (by protonation of the dpp) of a charge transfer band (around 470 nm) resulting from the  $\pi$ -electron donor-acceptor noncovalent interaction.

L26 ANSWER 37 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:670317 HCAPLUS

DOCUMENT NUMBER: 121:270317

TITLE: Electrochemically Triggered Swinging of a [2]-Catenate

AUTHOR(S): Livoreil, Aude; Dietrich-Buchecker, Christiane O.; Sauvage, Jean-Pierre

CORPORATE SOURCE: Faculte de Chimie, Universite Louis Pasteur,

Strasbourg, 67000, Fr.

SOURCE: Journal of the American Chemical Society (1994),

116(20), 9399-400

CODEN: JACSAT; ISSN: 0002-7863

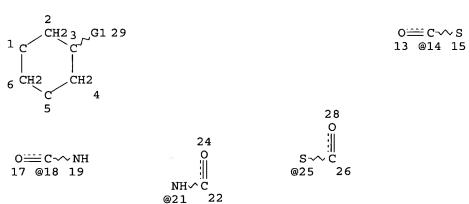
DOCUMENT TYPE: Journal LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The synthesis of an asym. copper(I) [2]-catenate is reported. [CuLL'] (L = I, L' = II) consists of two interlocking rings, with one of the two rings contains two coordination sites. As a consequence, two possible bonding modes between the metal center and the ligand with interlocking rings can be obtained. By changing the copper atom oxidation state, a complete rearrangement of the organic backbone is obtained which corresponds to the sliding motion of one ring within the other. The process is perfectly reversible and can be extremely slow (hours). Both forms of the same copper(II) state display very different spectro- and electrochem. properties.

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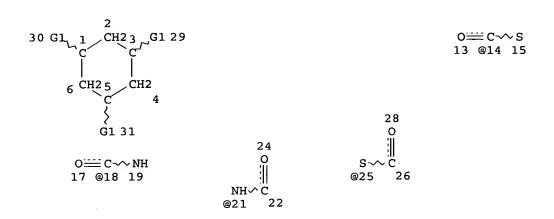
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NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

L14 56598 SEA FILE=REGISTRY SSS FUL L12

L17 STR



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GRAPH ATTRIBUTES:

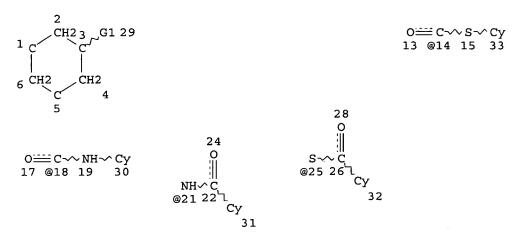
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NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L18 167 SEA FILE=REGISTRY SUB=L14 SSS FUL L17

L20 STR



VAR G1=14/18/21/25 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 23

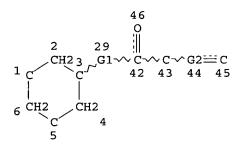
STEREO ATTRIBUTES: NONE

L21 STR

VAR G1=N/S REP G2=(0-20) C NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE L22 STR



VAR G1=S/N REP G2=(0-20) C NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L23	145 SEA FILE:	REGISTRY SUB=L1	8 SSS FUI	L L21 OR L22 OR L20
L24	60 SEA FILE	HCAPLUS ABB=ON	PLU=ON	L23
L25	39 SEA FILE:	HCAPLUS ABB=ON	PLU=ON	("LIVOREIL A"/AU OR "LIVOREIL
	AUDE"/AU)	1		
L26	37 SEA FILE:	HCAPLUS ABB=ON	PLU=ON	L25 NOT L24
L27	TRANSFER	PLU=ON L26 1-	37 RN :	413 TERMS
L28	413 SEA FILE=	REGISTRY ABB=ON	PLU=ON	L27
L29	2 SEA FILE=	REGISTRY ABB=ON	PLU=ON	(L28 AND L14) NOT L23
L30	10 SEA FILE=	HCAPLUS ABB=ON	PLU=ON	L29
L31	5 SEA FILE:	HCAPLUS ABB=ON	PLU=ON	L30 NOT (L24 OR L26)

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L31 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:650965 HCAPLUS

DOCUMENT NUMBER: 141:179215

TITLE: Nonfluid cosmetic makeup compositions containing a

waxy phase

INVENTOR(S): Ferrari, Veronique

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Fr. Demande, 27 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		<b>-</b>		
FR 2850867	A1	20040813	FR 2003-1461	20030207
PRIORITY APPLN. INFO.:			FR 2003-1461	20030207

OTHER SOURCE(S): MARPAT 141:179215

AB A nonfluid cosmetic composition for makeup composition comprises an oily phase, 6-25% a nonpolar waxy phase, and 0.5-10% a diamide. Thus, a rouge composition contained polyethylene wax 15, N,N'-bis(dodecanoyl)-1,2-diaminocyclohexane 2, pigments 8, perfumes 0.2, preservatives qs, and Parleam qs to 100 g.

IT 390747-75-8

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (nonfluid cosmetic makeup compns. containing waxy phase)

RN 390747-75-8 HCAPLUS

CN Dodecanamide, N, N'-1, 3-cyclohexanediylbis- (9CI) (CA INDEX NAME)

$$Me^{-(CH_2)_{10}-C-NH}$$
  $NH^{-C^{-(CH_2)_{10}-Me}}$ 

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:203152 HCAPLUS

DOCUMENT NUMBER: 140:258619

TITLE: Cosmetic composition containing oils, a rheological

agent and a particulate phase

INVENTOR(S): Blin, Xavier; Ferrari, Veronique

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: Fr. Demande, 21 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844186	A1	20040312	FR 2002-11095	20020906

EP 1405625 Α1 20040407 EP 2003-20174 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK US 2004126350 A 1 20040701 US 2003-656146 JP 2004262919 A2 20040924 JP 2003-315977 20030908 PRIORITY APPLN. INFO.: FR 2002-11095 A 20020906 US 2002-410955P P 20020917

AB A cosmetic composition comprises in a physiol. acceptable medium, at least a Ph silicone oil of high viscosity, at least a nonvolatile hydrocarbon oil having a mol. weight higher than 500 g/Mol and/or an index of refraction at 20°C higher than 1.440, at least a rheol. agent and a particulate phase. The composition has good brightness, and comfort. A lipstick contained di-isostearyl malate q.s. 100, Ph trimethyltrisiloxane (20 cSt) (Dow Corning DC556) 18, Ph tri-Me trisiloxane (1000 cSt) (Belsil PDM 1000) 27, microcryst. wax 10, C30-45 alkyl dimethicone 2.5, a mixture of lauric, myristic, palmitic, and stearic acid triglycerides, (50/20/10/10) (Softisan 100) 10, Red 7 0.26, Red 21, 0.06 black iron oxide 0.09, brown iron oxide 2,1 mica titanium oxide 1.8%.

IT 99063-92-0, 1,3,5-Cyclohexanetricarboxamide
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(cosmetic composition containing oils, rheol. agent and particulate phase)

RN 99063-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ \parallel & \parallel & \parallel \\ C-NH_2 & \\ \hline C-NH_2 & \\ \parallel & O \end{array}$$

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:490016 HCAPLUS

DOCUMENT NUMBER: 135:227474

TITLE: Anionic Polymerization of an Acrylonitrile Trimer

Studied by Photoelectron Spectroscopy

AUTHOR(S): Fukuda, Yuji; Ichihashi, Masahiko; Terasaki, Akira;

Kondow, Tamotsu; Osoda, Kazuhiko; Narasaka, Koichi

CORPORATE SOURCE: Department of Chemistry School of Science, The

University of Tokyo, Bunkyo-ku Tokyo, 113-0033, Japan

SOURCE: Journal of Physical Chemistry A (2001), 105(30),

7180-7184

CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB A photoelectron spectrum of an acrylonitrile (AN:CH2:CHCN) trimer anion, (AN)3-, produced by electron impact on an acrylonitrile cluster was measured, and was compared with that of a mol. anion of 1,3,5-cyclohexanetricarbonitrile (c-HTCN) in the triequatorial form, which was first synthesized in the present experiment A comparison of the vertical

detachment energies of (AN)3- and the mol. anion lead us to conclude that (AN)3- is assigned as one of the stereoisomers (diaxial form) of c-HTCN (-) on the basis of our previous studies refs. 13, 14, and 20-22 [Tsukuda, T.; Kondow, T. J. Chemical Phys. 1991, 95, 6989. Tsukuda, T.; Kondow, T. J. Am. Chemical Society 1994, 116, 9555. Ichihashi, M.; Tsukuda, T.; Nonose, S.; Kondow, T. J. Phys. Chemical 1995, 99, 17354. Fukuda, Y.; Tsukuda, T.; Terasaki, A.; Kondow, T. Chemical Phys. Lett. 1995, 242, 121. Fukuda, Y.; Tsukuda, T.; Tsukuda, T.; Terasaki, A.; Kondow, T. Chemical Phys. Lett. 1996, 260, 423.]. 99063-92-0P, 1,3,5-Cyclohexanetricarboxamide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(in preparation and anionic polymerization of acrylonitrile trimer studied

by

IT

photoelectron spectroscopy)

RN 99063-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \parallel & \parallel \\ H_2N-C & C-NH_2 \\ \hline \\ C-NH_2 \\ \parallel \\ O \end{array}$$

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1959:105200 HCAPLUS

DOCUMENT NUMBER: 53:105200
ORIGINAL REFERENCE NO.: 53:18859d-f

TITLE: Reaction between substituted malonic esters and

methylene bromide. II

AUTHOR(S): Eberson, Lennart CORPORATE SOURCE: Univ. Lund, Swed.

SOURCE: Acta Chemica Scandinavica (1958), 12, 731-6

CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal LANGUAGE: English

The reaction between (EtO2C)2CHCH(CO2Et)2 and CH2Br2 or CH2I2 occurred in boiling alc. solution contrary to the belief [Kotz and Stalmann, J. prakt. Chemical 68, 156(1903)] that temps. above 130° were required to obtain reasonable yields. The product (after 20 hrs. refluxing) consisted solely of 71% tetra-Et 1,1,2,2-cyclopropanetetracarboxylate, m. 41-2° (absolute Et2O-petr. ether); no trace of Et2CO3 could be detected. Repetition of the reaction with (EtO2C)2CHCH2CH(CO2Et)2 gave largely CH2:C(CO2Et)2 and gave only tarry products on acid or alkaline hydrolysis. On raising the reaction temp to 100° for 30 hrs. pentaethyl 1,1,3,3,5-cyclohexane pentacarboxylate, b4 210-15° [tetraacid, m. 205-10° (decomposition) (Me2CO)], resulted and gave on alkaline hydrolysis the corresponding pentaacid, m. 180-4° (decomposition) (glacial AcOH), and on acid hydrolysis 1,3,5-cyclohexane tricarboxylic acid, m. 212-15° (C6H6-Me2CO) [triamide m. 286-9° (decomposition) (H2O); tri-Me ester m. 43-5° (petr. ether)]. A small amount of Et2CO3, b50 50-60°,

was isolated. With (EtO2C)2CHCH2CH2CH(CO2Et)2 and (EtO2C)2CH(CH2)3CH(CO2Et)2 the principal products were tetra-Et 1,1,3,3-cyclopentanetetracarboxylate, m. 185-90° (decomposition) (H2O), and tetra-Et 1,1,3,3-cyclohexanetetracarboxylate, m. 210-20° (decomposition) (H2O), resp., confirming the results of previous investigations and again manifesting the effect that accommodation of substituents at the ends of a closing C chain facilitates ring formation.

RN 99063-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & O \\
H_2N-C & C-NH_2 \\
\hline
C-NH_2 \\
0
\end{array}$$

L31 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1955:69098 HCAPLUS

DOCUMENT NUMBER: 49:69098

ORIGINAL REFERENCE NO.: 49:13242d-i,13243a-h

TITLE: Attempted syntheses of nitrogen analogs of adamantane

AUTHOR(S): Newman, Melvin S.; Lowrie, Harman S.

CORPORATE SOURCE: Ohio State Univ., Columbus

SOURCE: Journal of the American Chemical Society (1954), 76,

4598-600

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB Attempts to prepare N analogs of adamantane from 1,3,5-trisubstituted cyclohexanes failed. A number of these cyclohexanes were related in configuration, postulated to be cis. 1,3,5-C6H3(CO2Me)3, white needles,

m. 145-6° (from MeOH), reduced and distilled gave tri-Me

1,3,5-cyclohexanetricarboxylate (I), semisolid crystalline mixture of isomers, which was recrystd. 3 times from Et2O at -70°; in the best of

several runs, 33.3 g. mixture gave 20.6 g., solid I, m. 48.0-9.0°

(all m. ps. are corrected); addnl. crops could be obtained from the mother liquors. Solid I (30.0 g.) reduced with LiAlH4 slurried in Et20, the

mixture acidified with dilute H2SO4, saturated with Na2SO4, and extracted continuously

12 days with Et2O, the extract diluted with MeOH, the solution passed through Al2O3 to remove traces of acid, and the solvents removed gave 14.6 g. oily yellow solid, which recrystd. 3 times from Me2CO gave 1,3,5-cyclohexanetrimethanol (II), white rods, m. 101.0-2.0°. Isomeric mixture (43.8 g.) of I reduced in the same way gave 32.5 g. oily solid which recrystd. from Me2CO gave 8.4 g. II, m. 97-100°; the mother liquor

evaporated to dryness, the residual oil refluxed with dilute aqueous NaOH, and

solution saturated with Na2SO4 and extracted with Et2O in the usual manner yielded

10.6 q. II, m. 95-100°. II (2.10 g.) in dry pyridine treated 3 hrs. at -5 to 0° with MeSO2Cl, the mixture worked up in the cold, the resulting yellow solid dissolved in Me2CO, the solution passed through Norit A and the solvent removed with air gave 4.4 g. trimethanesulfonate (III) of II, white crystals, m. 125.5-6.5° (recrystd. twice from Me2CO-Et2O, m. 126.8-7.4°). Crude III (35 g.), m. 108-18°, shaken overnight in a steel bomb with 500 cc. dioxane and 0.6 mole dry NH3, the mixture heated slowly to 85° for 24 hrs., cooled, treated with 0.2 mole NH3, heated 24 hrs. at 95°, cooled, poured into dilute H2SO4, steam distilled to remove the dioxane, made strongly basic, and again steam distilled, the distillate collected in dilute HCl until it was no longer basic, the resulting solution evaporated, the yellow-white solid residue dried and extracted once with Me2CO to remove the yellow color and 3 times with CHCl3, the CHCl3 extract evaporated, and the white powdery residue (0.42 g., 2.8%) recrystd. from EtOH-PhMe gave a compound C9H15N (IV).HCl, white crystals, insol. in Me2CO, but readily soluble in CHCl3. IV.HCl treated 12 hrs. at 95° with aqueous HNO2 was recovered unchanged. IV.HCl sublimed at 180-200° before melting in an open tube and melted above 400° in a sealed tube. Alkaline aqueous KMnO4 was immediately discolored by the addition of 0.10 g. IV.HCl in base; the solution treated with KMnO4 until

the color persisted, refluxed 1 hr., and distilled gave less than 5 mg. white powder identified as NH4Cl. IV.HCl in CHCl3 treated dropwise with Br in CCl4 until the Br color persisted, the solvents removed with air, the orange solid residue dissolved in absolute EtOH, the solution diluted with ligroine

(b. 90-7°), and the yellow precipitate washed with a small amount of Me2CO and recrystd. from boiling Me2CO deposited 2 crystal forms which were separated manually, washed with cold Me2CO, and dried to give 20 mg. compound C9H15Br2N, long needles, fairly soluble in Me2CO; and 15 mg. IV.HBr, small cubes, rather insol. in Me2CO. A small amount of IV.HCl dissolved in HBr and the solution evaporated gave IV.HBr. I (20.5 g.) refluxed 2-3 hrs. with dilute

NaOH, the solution concentrated, acidified with H2SO4, saturated with Na2SO4, and extracted

continuously 12 hrs. with Et2O, and the extract evaporated gave 18.0 g. 1,3,5-cyclohexanetricarboxylic acid-1.5H2O (V.1.5-H2O), white powdery solid, m. 208-13°, which gave, recrystn. 3 times from Me2CO-C6H6, V, white needles, m. 215-18°. V (1.30 g.) treated with CH2N2 gave 1.22 g. solid, m. 43-7°, which distilled and recrystd. from Et2O at -70° gave I, fine needles, m. 48-9°. V treated with SOCl2, the resulting acid chloride dissolved in C6H6, the solution added to 28% NH4OH, the aqueous layer cooled and filtered, and the filter residue recrystd. twice from H2O yielded 1,3,5-cyclohexanetricarboxamide (VI), white crystals, m. 287.5-8.5° (decomposition) with softening at 283.5°. VI (1.24 g.) sublimed during 6 hrs. at 285° gave 0.81 g. (78%) sublimate (collected in several fractions), m. between 210 and 240° in 20° ranges; this sublimate boiled with EtOH in which it was rather insol., the EtOH removed, and the residue recrystd. twice from Me2CO gave VII (R = CN), white crystals, m. 239-43° with darkening after softening at 230-1°. V (1.3 g.) in 5 cc. 28% NH40H evaporated to dryness, the residue pyrolyzed at 270-300°, and the white solid sublimate dried in vacuo gave 0.90 g. material, m. 230-50° (decomposition) with softening at 190-220°, which recrystd. twice from EtOH-PhMe yielded a compound C9H11NO4 (VIII), white poorly formed crystals, m. 244-7° (decomposition) with softening at 240-4°. V (6.1 g.) gave similarly 4.2 g. material which was sublimed and collected in fractions; 1 fraction resublimed at 195° and 0.1 mm. gave white powdery crystals, m. 215-33° (decomposition) with softening at 204°; another fraction recrystd. twice from EtOH-PhMe and then

sublimed at 195° and 0.1 mm. gave a white powder, m. 227-54° (decomposition) with softening at 223°. The various fractions of VIII, which was a mixture of IX and VII (R = CO2H), showed initially neutral equivs. of 280-300 which dropped to a final value of 108-14 when excess base was added. A portion of the material upon which the neutral equivalent had been taken boiled with dilute aqueous NaOH, the mixture acidified with HCl

evaporated to dryness, the residue extracted with Me2CO, the extract evaporated, and the

residue recrystd. from EtOH-PhMe gave V, white needles, m. 211-15°. V treated with CH2N2 gave I, clear needles, m. 48-9°. V (10.8 g.) treated with NH4OH, the mixture evaporated, and the residue pyrolyzed gave 6.6 g. product having the same m.p. range and infrared spectrum as the sublimates of VIII; a 3-g. sample let stand 2 days with SOCl2, the mixture refluxed a short time and evaporated in vacuo, and the residue sublimed at 35 mm. gave 0.9 g. VII (R = COCl) (X), white needles, m. 170-80° (rapid heating). X (0.3 g.) in CHCl3 previously saturated with NH3 let stand 1 hr., filtered, and evaporated, and the residue sublimed and then recrystd. from Me2CO-C6H6 gave 0.05 g. tan crystals, m. 260-5°; the mother liquor evaporated gave VII (R = CN), white crystals, m. 207-20°.

RN 99063-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)

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